Supporting Information

Copper-Catalyzed Aerobic Oxidative Synthesis of Aromatic Carboxylic Acids

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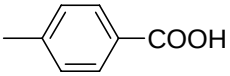
General experimental procedures

All reagents and solvents were obtained from commercial suppliers and used without further purification. CuI and CuBr were purchased from Alfa Aesar, and other reagents were purchased from Beijing Ouhe Technology Ltd. Co.. All reagents were weighed and handled in air at room temperature. Flash chromatography was performed on silica gel (200 ~ 300 mesh). Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) in the solvent of $CDCl_3$ as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CHCl_3$ at 7.24 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm) or using tetramethylsilane (TMS) in the solvent of DMSO-d_6 as the internal standard (^{1}H NMR: TMS at 0.00 ppm, DMSO at 2.50 ppm; ^{13}C NMR: DMSO at 40.0 ppm).

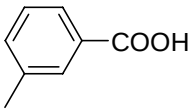
General procedure for synthesis of aromatic carboxylic acids (3a-u). Synthesis of aromatic carboxylic acids was performed under two conditions. For method **A**, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with CuI (0.2 mmol, 38 mg), L-proline (0.2 mmol, 23 mg), Cs_2CO_3 (3 mmol, 978 mg for synthesis of **3o** and **3p**; 2 mmol, 652 mg for synthesis of others), aryl halide (1 mmol), malononitrile (2 mmol, 132 mg), DMSO (2 mL) (without previous anhydrous procedure), and the tube with an air balloon (1 atm.) was sealed and put into a pre-heated oil bath at 140 °C for 48 h. After the resulting solution was cooled to room temperature, DMSO was removed under rotary evaporation, and then 4 mL of HCl (1 M) was added to the residue (pH = 2 ~ 3). The solution was extracted with ethyl acetate (4 × 5 mL), the combined organic phase was concentrated, and the residue was purified by column chromatography on silica gel to provide the desired product (Note: for product **3o** or **3p**, DMSO was removed under rotary evaporation, and then 4 mL of HCl (1 M) was added to the residue (pH = 2 ~ 3). Water was removed under rotary evaporation, and the residue was purified by column chromatography on silica gel to provide the desired product). For method **B**, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with CuI (0.2 mmol, 38 mg), L-proline (0.2 mmol, 23 mg), Cs_2CO_3 (3 mmol, 978 mg for synthesis of **3o** and **3p**; 2 mmol, 652 mg for synthesis of others), and aryl halide if a solid (1 mmol). The tube was evacuated twice

and back-filled with nitrogen. Aryl halide as a liquid (1 mmol), malononitrile (2 mmol, 132 mg), and DMSO (1 mL) were sequentially added at room temperature under a stream of nitrogen, and the tube was sealed and put into a pre-heated oil bath at 130 °C for 24 h under a positive pressure of nitrogen, and the tube was opened to allow air in, and the following reaction in air was performed at 140 ^{o}C for 12 h. After the resulting solution was cooled to room temperature, the work-up procedure was similar to Method **A**.



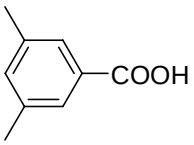
3a

4-Methylbenzoic acid (3a).[1] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 181-182 ^{o}C (lit.[1] 181-182 ^{o}C). ^{1}H NMR ($CDCl_3$, 600 MHz, ppm) δ 12.59 (s, br, 1H), 7.93 (d, 2H, J = 8.3 Hz), 7.18 (d, 2H, J = 8.3 Hz), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz, ppm) δ 172.7, 144.8, 130.4, 129.4, 126.7, 21.8. ESI-MS $[M+H]^+$ m/z 137.2.



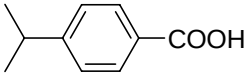
3b

3-Methylbenzoic acid (3b).[2] Eluent petroleum ether/ethyl acetate (2:1). White solid. mp 112-114 ^{o}C (lit.[2] 111-112 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 11.85 (s, br,1H), 7.94-7.92 (m, 2H), 7.44-7.37 (m, 2H), 2.47 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.7, 138.4, 134.7, 130.8, 129.3, 128.5, 127.5, 21.4. ESI-MS $[M+H]^+$ m/z 137.5.



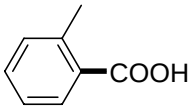
3c

3,5-Dimethylbenzoic acid (3c).[3] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 165-166 ^{o}C (lit.[3] 161-162 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 11.26 (s, br,1H), 7.79 (s, 2H), 7.25 (m, 1H), 2.38 (s, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.6, 138.3, 135.6, 129.2, 128.0, 21.2. ESI-MS $[M-H]^-$ m/z 149.5.



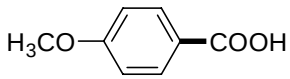
3d

4-Isopropylbenzoic acid (3d).[4] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 114-115 ^{o}C. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 12.76 (s, br,1H), 7.86 (d, 2H, J = 7.9 Hz), 7.25 (d, 1H, J = 7.9 Hz), 2.96 (m, 1H, J = 6.8 Hz), 1.19 (d, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.4, 155.5, 130.5, 127.0, 126.7, 34.4, 23.8. ESI-MS $[M+H]^+$ m/z 165.2.



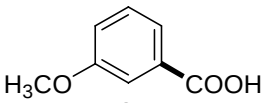
3e

2-Methylbenzoic acid (3e).[5] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 101-102 ^{o}C (lit.[5] 106.0-105.5 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 12.84 (s, br, 1H), 7.87 (d, 1H, J = 7.9 Hz), 7.52-7.47 (m, 1H), 7.36-7.31 (m, 2H), 2.56 (s, 3H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 169.2, 139.5, 132.2, 132.0, 131.0, 130.7, 126.3, 21.7. ESI-MS $[M-H]^-$ m/z 136.5.



3f

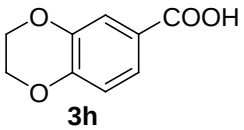
4-Methoxybenzoic acid (3f).[6] Eluent petroleum ether/ethyl acetate (2:1). White solid. mp 184-185^{o}C (lit.[6] 186-187 ^{o}C). ^{1}H NMR (DMSO-d_6, 600 MHz, ppm) δ 12.63 (s, br, 1H), 7.89 (d, 2H, J = 8.9 Hz), 7.01 (d, 2H, J = 8.9 Hz), 3.81 (s, 3H). ^{13}C NMR (DMSO-d_6, 150 MHz, ppm) δ 167.5, 163.3, 131.7, 123.5, 114.3, 55.9. ESI-MS $[M-H]^-$ m/z 151.4.



3g

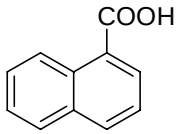
3-Methoxybenzoic acid (3g).[7] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 107-108 ^{o}C (lit.[7] 107-109 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 7.72 (d, 1H, J = 7.9 Hz), 7.63 (s, 1H), 7.39 (t, 1H, J = 7.9 Hz), 7.18 (d, 1H, J = 7.9 Hz), 3.88 (s,

3H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.3, 159.7, 130.7, 129.6, 122.8, 120.6, 114.5, 55.6. ESI-MS $[M-H]^-$ m/z 151.5.



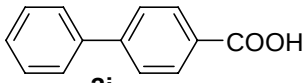
3h

2,3-Dihydrobenzo[*b*][1,4]dioxine-6-carboxylic acid (3h).[8] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 135-137 ^{o}C (lit.[8] 136 ^{o}C). ^{1}H NMR (DMSO-d_6,300 MHz, ppm) δ 12.74 (s, br,1H), 7.49 (dd, 1H, J = 8.3 Hz), 7.43 (d, 1H, J = 2.1 Hz), 7.00 (d, 1H, J = 8.6 Hz), 4.33 (dd, 4H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 167.2, 148.0, 143.5, 124.3, 123.5, 118.7, 117.6, 64.9, 64.4. ESI-MS $[M-H]^-$ m/z 179.7.



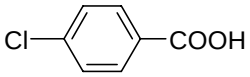
3i

1-Naphthoic acid (3i).[9] Eluent petroleum ether/ethyl acetate (2:1). White solid. mp 154-155 ^{o}C (lit.[9] 162 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 9.10 (d, 1H, J = 8.9 Hz), 8.42 (d, 1H, J = 7.2 Hz), 8.11 (d, 1H, J = 7.9 Hz), 7.93 (d, 1H, J = 8.3 Hz), 7.68 (t, 1H, J = 8.3 Hz), 7.60-7.54 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.9, 134.7, 131.9, 131.8, 128.8, 128.2, 126.3, 126.0, 125.8, 124.6. ESI-MS $[M-H]^-$ m/z 171.5.



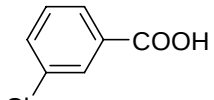
3j

[1,1'-Biphenyl]-4-carboxylic acid (3j).[10] Eluent petroleum ether/ethyl acetate (3:1). Yellow solid. mp 224-226 ^{o}C (lit.[10] 224-225 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 12.98 (s, br, 1H), 8.02 (d, 2H, J = 8.3 Hz), 7.80 (d, 2H, J = 8.3 Hz), 7.74 (d, 2H, J = 8.6 Hz), 7.50 (t, 2H), 7.42 (t, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 167.7, 144.8, 139.6, 130.5, 130.1, 129.6, 128.8, 127.5, 127.4. ESI-MS $[M-H]^-$ m/z 279.6.



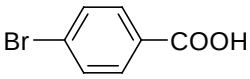
3k

4-Chlorobenzoic acid (3k).[11] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 250 ^{o}C (lit.[11] 243 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.17 (s, br, 1H), 7.95 (d, 2H, J = 7.9 Hz), 7.57 (d, 1H, J = 7.9 Hz). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 166.5, 137.8, 131.3, 129.6, 128.7. ESI-MS $[M-H]^-$ m/z 155.6.



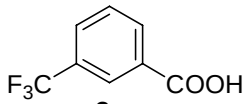
3l

3-Chlorobenzoic acid (3l).[12] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 137-138^{o}C (lit.[12] 155.8-156.8 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.38 (s, br, 1H), 7.95 (m, 2H), 7.75 (d, 1H), 7.60 (m, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 166.6, 133.9, 133.5, 133.2, 131.2, 129.4, 128.4. ESI-MS $[M-H]^-$ m/z 155.5.



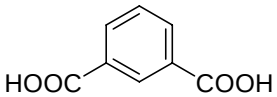
3m

4-Bromobenzoic acid (3m).[13] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 256-257 ^{o}C (lit.[13] 252-254^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.17 (s, br,1H), 7.87 (d, 2H, J = 8.6 Hz), 7.71 (d, 2H, J = 8.6 Hz). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 167.1, 132.2, 131.8, 130.5, 127.4. ESI-MS $[M-H]^-$ m/z 201.0.



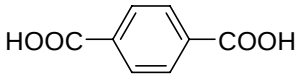
3n

3-(Trifluoromethyl)benzoic acid (3n).[14] Eluent petroleum ether/ethyl acetate (3:1). White solid. mp 180-182 ^{o}C (lit.[14] 180-183 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.49 (s, br, 1H), 8.22 (d, 1H, J = 7.9 Hz), 8.17 (s, 1H), 7.99 (d, 2H, J = 7.9 Hz), 7.76 (t, 1H, J = 7.9 Hz). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 166.5, 133.7, 132.4, 130.6, 129.9 (q, J = 33.0 Hz),, 126.0, 122.5. ESI-MS $[M+H]^+$ m/z 191.0.



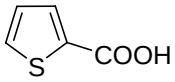
3o

Isophthalic acid (3o).[15] Eluent petroleum ether/ethyl acetate (1:1). White solid. mp 280 ^{o}C (lit.[15] 345 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.26 (s, br, 2H), 8.49 (s, 1H), 8.17 (d, 2H, J = 7.9 Hz), 7.65 (d, 1H, J = 7.9 Hz). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 167.1, 133.9, 131.8, 130.5, 129.7. ESI-MS [M-H]$^{-}$ m/z 165.6..



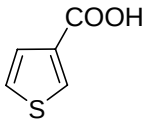
3p

Terephthalic acid (3p).[16] Eluent ethyl acetate. White solid. mp 280-300^{o}C (lit.[16] 280-300 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.30 (s, br, 2H), 8.06 (s, 4H). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 167.2, 134.9, 129.9. ESI-MS [M-H]$^{-}$ m/z 165.6.



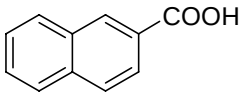
3q

Thiophene-2-carboxylic acid (3q).[17] Eluent petroleum ether/ethyl acetate (3:1).Yellow solid. mp 152-154 ^{o}C (lit.[17] 130-132 ^{o}C). ^{1}H NMR (DMSO-d_6, 300 MHz, ppm) δ 13.06 (s, br, 1H), 7.88 (d, 1H, J = 4.8 Hz), 7.74 (d, 1H, J = 3.8 Hz). ^{13}C NMR (DMSO-d_6, 75 MHz, ppm) δ 163.4, 135.2, 133.8, 133.7, 128.7. ESI-MS [M-H]$^{-}$ m/z 127.7.



3r

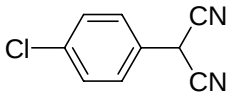
Thiophene-3-carboxylic acid (3q).[18] Eluent petroleum ether/ethyl acetate (3:1).Yellow solid. mp 139-140 ^{o}C (lit.[18] 137-138 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 11.72 (s, br, 1H), 8.23 (s, 1H), 7.57 (d, 1H, J = 4.1 Hz), 7.35 (d, 1H, J = 4.1 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 168.4, 134.8, 133.1, 128.3, 126.6. ESI-MS [M-H]$^{-}$ m/z 127.8.



3u

2-Naphthoic acid (3u).[19] Eluent petroleum ether/ethyl acetate (3:1). Yellow solid. mp 180-182 ^{o}C (lit.[19] 180-183 ^{o}C). ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 8.73 (s, 1H), 8.13

(d, 1H, *J* = 8.6 Hz), 8.00 (d, 1H, *J* = 7.89 Hz), 7.92. (m, 2H), 7.65-7.7.56 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 172.3, 136.0, 132.4, 132.3, 129.6, 128.8, 128.4, 127.9, 126.5, 126.9, 125.5. ESI-MS $[M-H]^-$ m/z 171.4.



4

2-(4-Chlorophenyl)malononitrile (4).[20] It was prepared via coupling of 1-chloro-4-iodobenzene with malononitrile according to the previous procedure.[20] Yellow solid. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 7.47 (dd, 4H), 5.06 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 137.0, 130.4, 128.7, 124.8, 111.5, 27.7. ESI-MS $[M-H]^-$ m/z 175.9.

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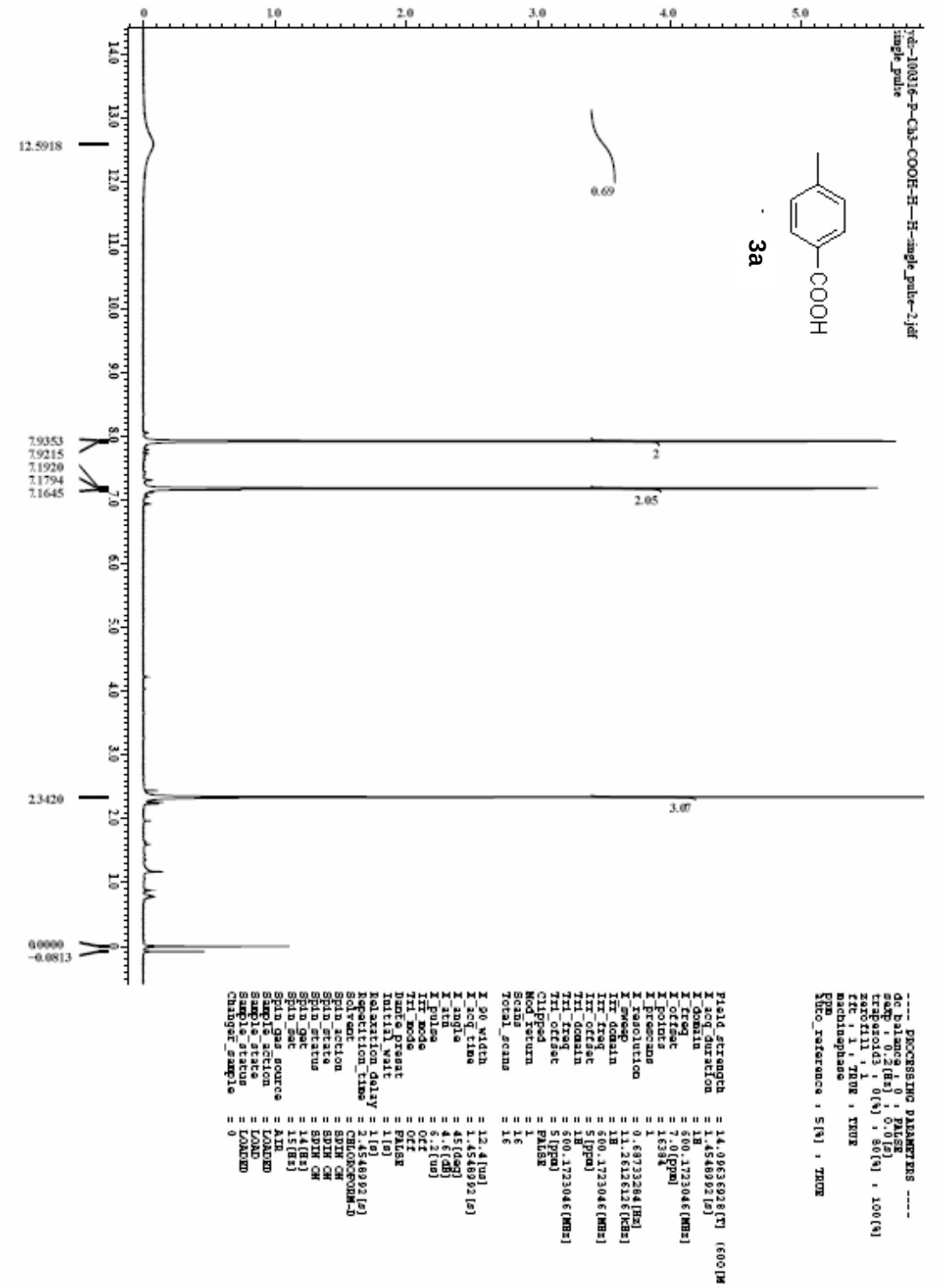
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COOH
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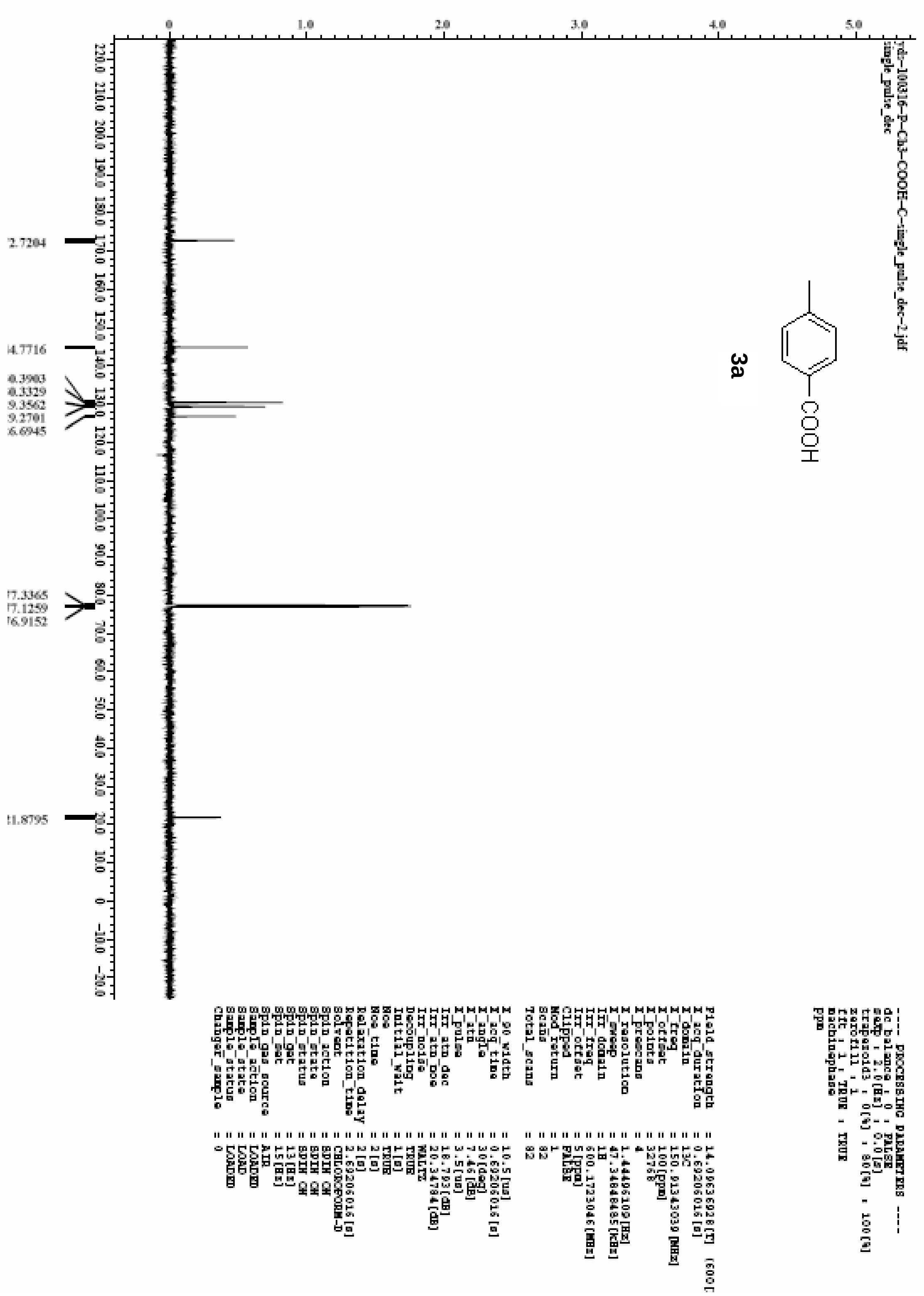
7.9353
7.9215
7.1920
7.1794
7.1645
2.3420
0.0000
-0.0813
0.69
2
2.05
3.07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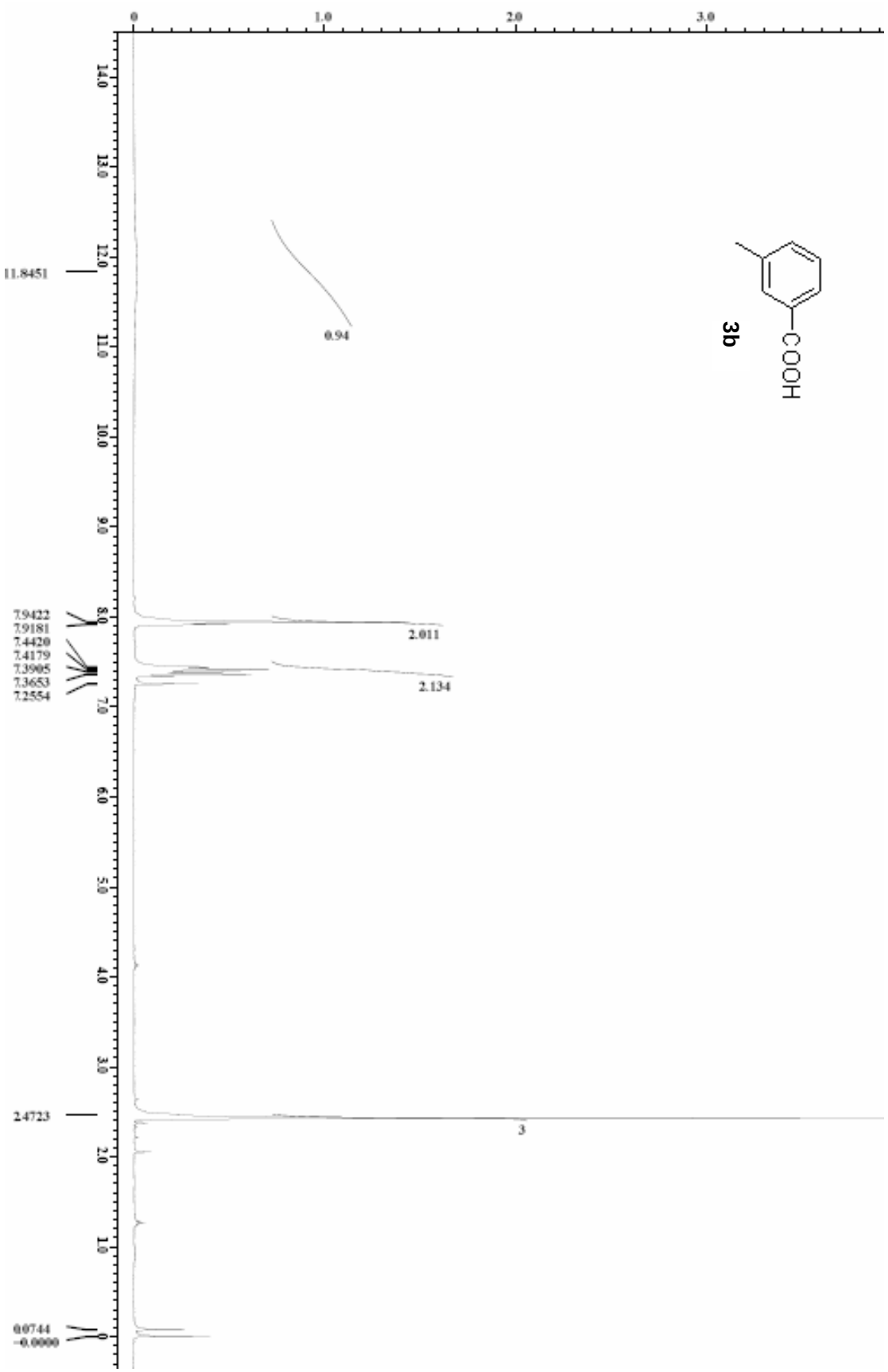
COOH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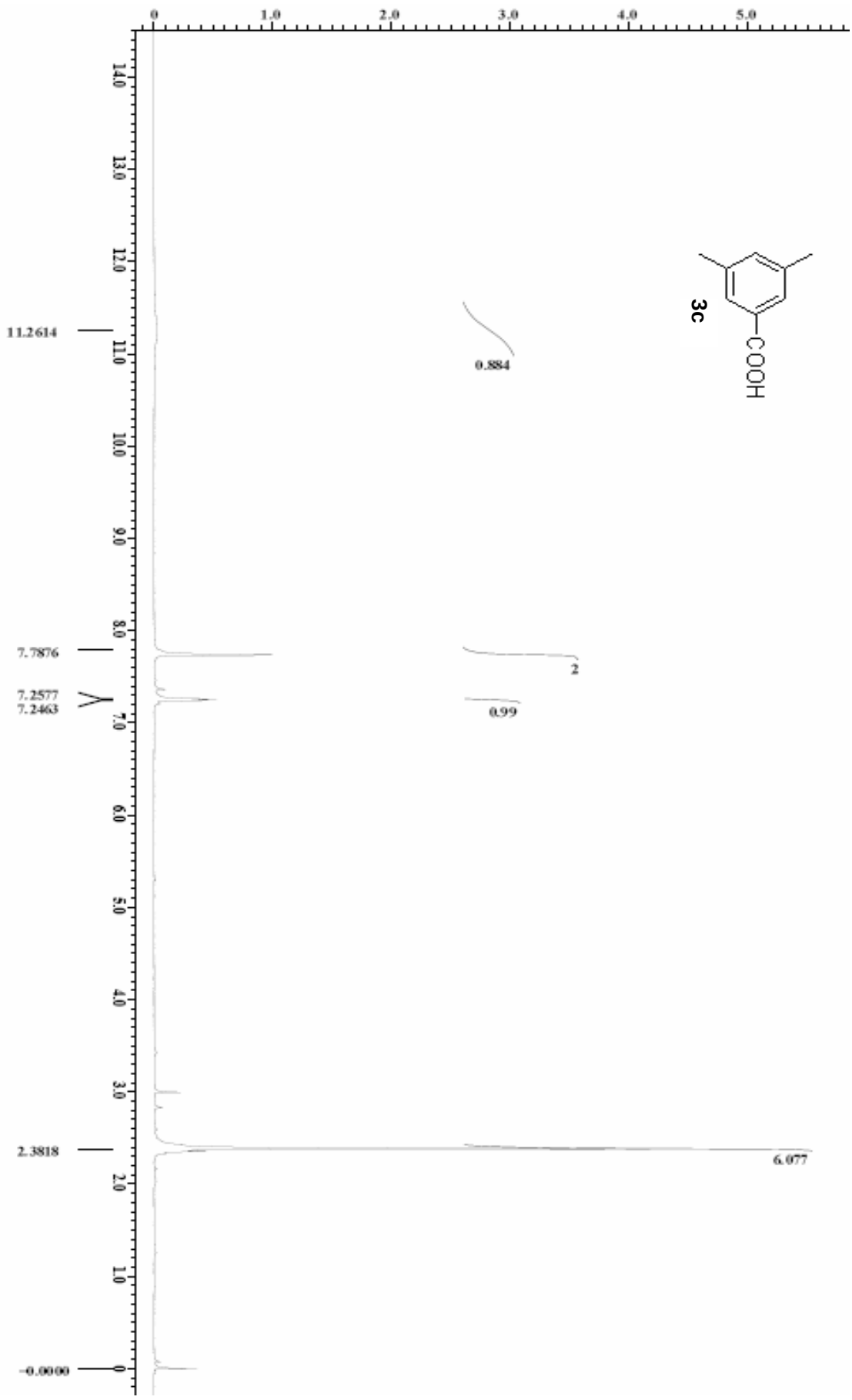
7.9422
7.9181
7.4420
7.4179
7.3905
7.3653
7.2554
2.4723
0.0744
-0.0000
0.94
2.011
2.134
3
3b
COOH


abundance
172.6887
138.4138
134.7138
130.8131
129.3121
128.4899
127.4764
77.5412
77.1205
76.6903
21.3629
COOH
3b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7.2463
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0.884
2
0.99
6.077
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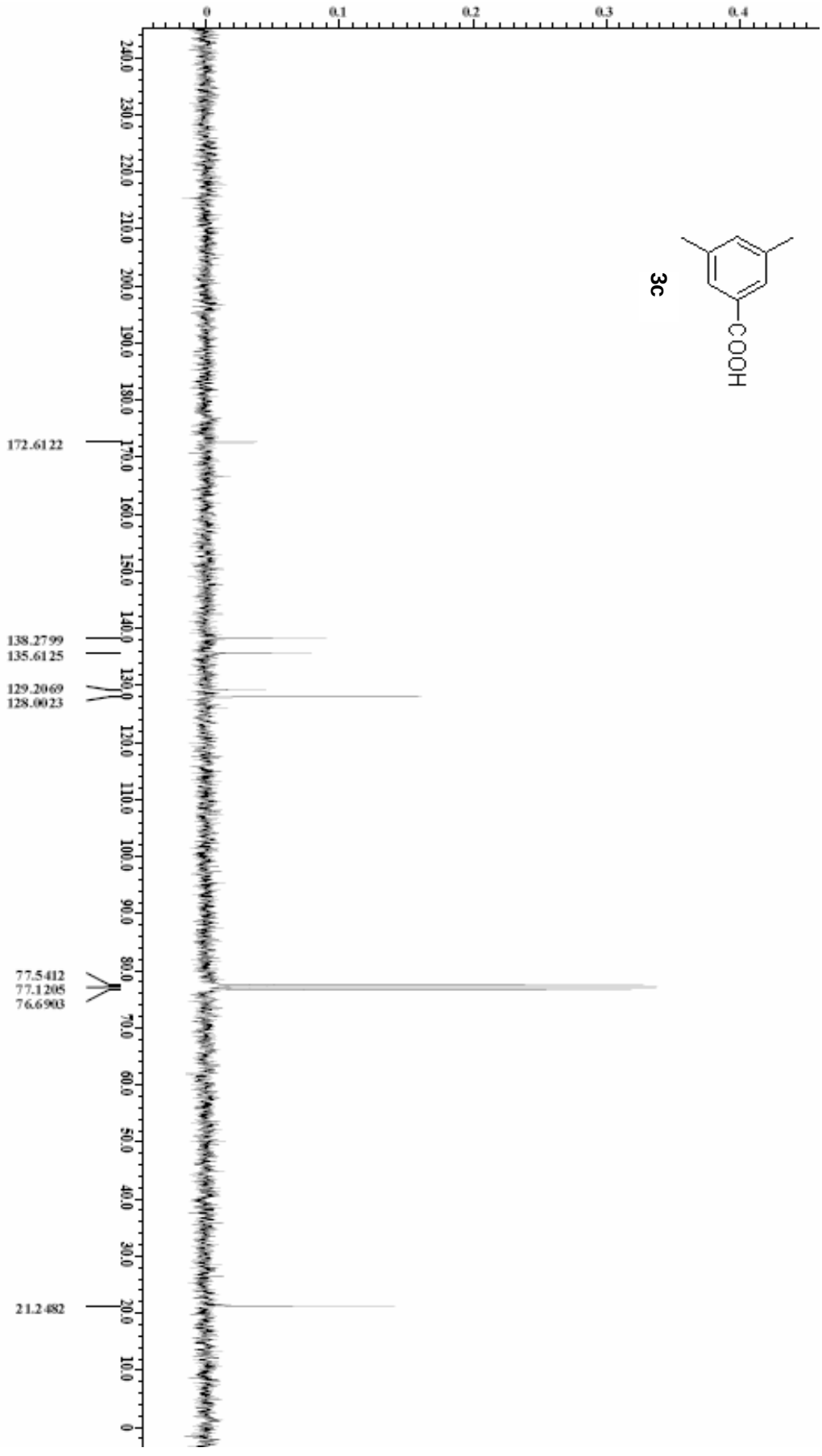
COOH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COOH
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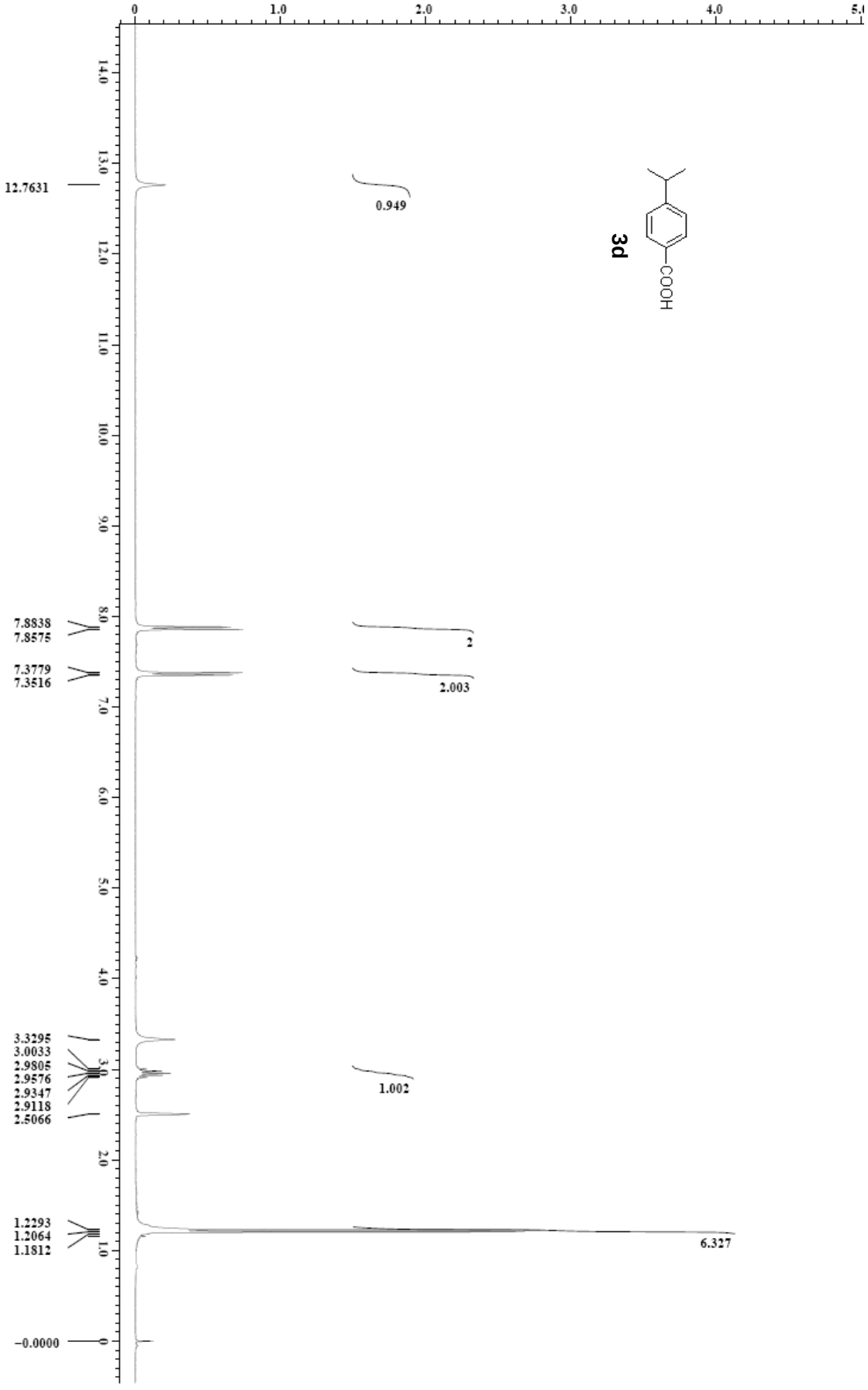
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7.8575
7.3779
7.3516
3.3295
3.0033
2.9805
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2.9118
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1.1812
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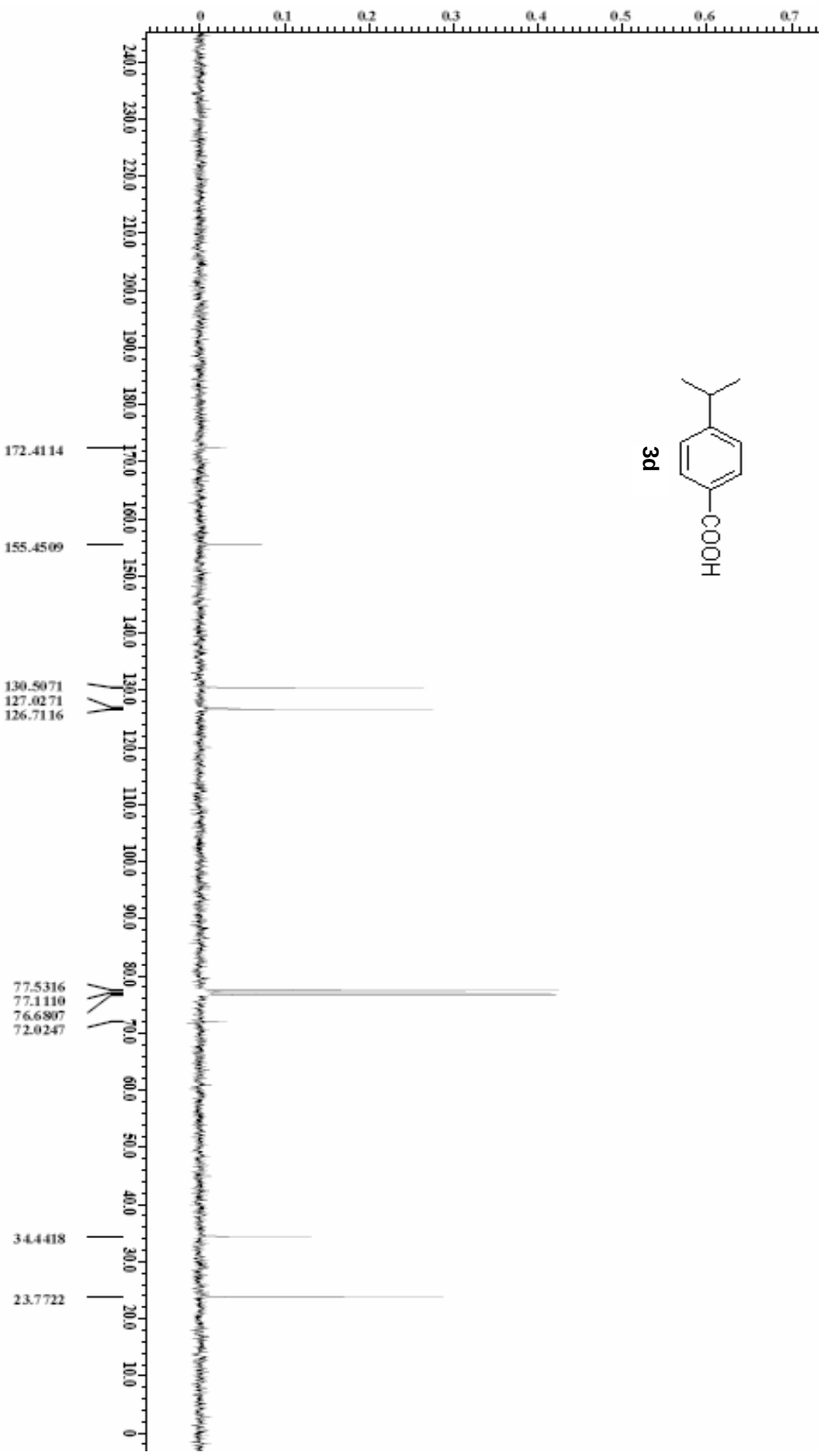
2
2.003
1.002
6.327
3d
COOH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130.5071
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126.7116
77.5316
77.1110
76.6907
72.0247
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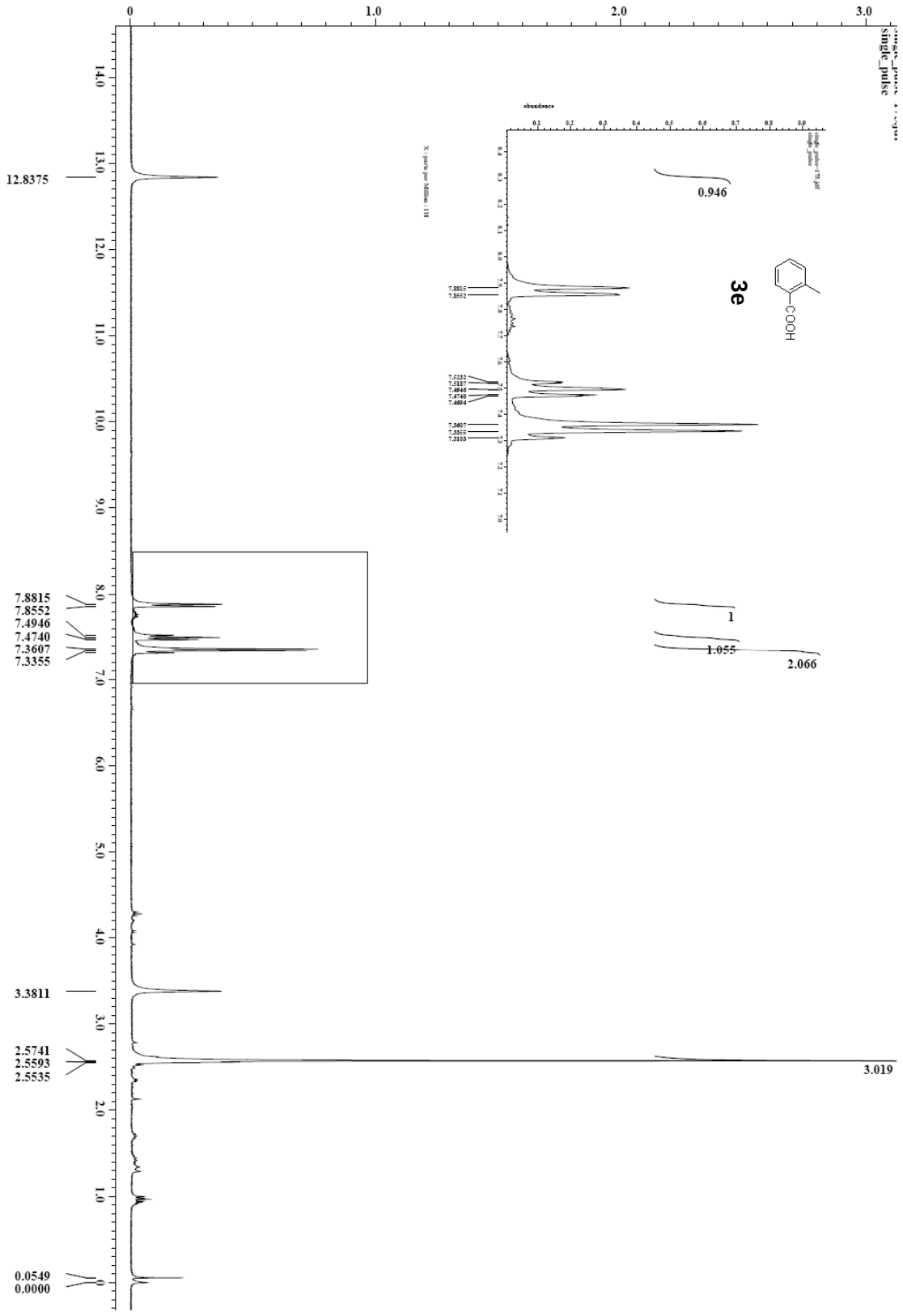
23.7722
3d
COOH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7.8552
7.4946
7.4740
7.3607
7.3355
3.3811
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0.0549
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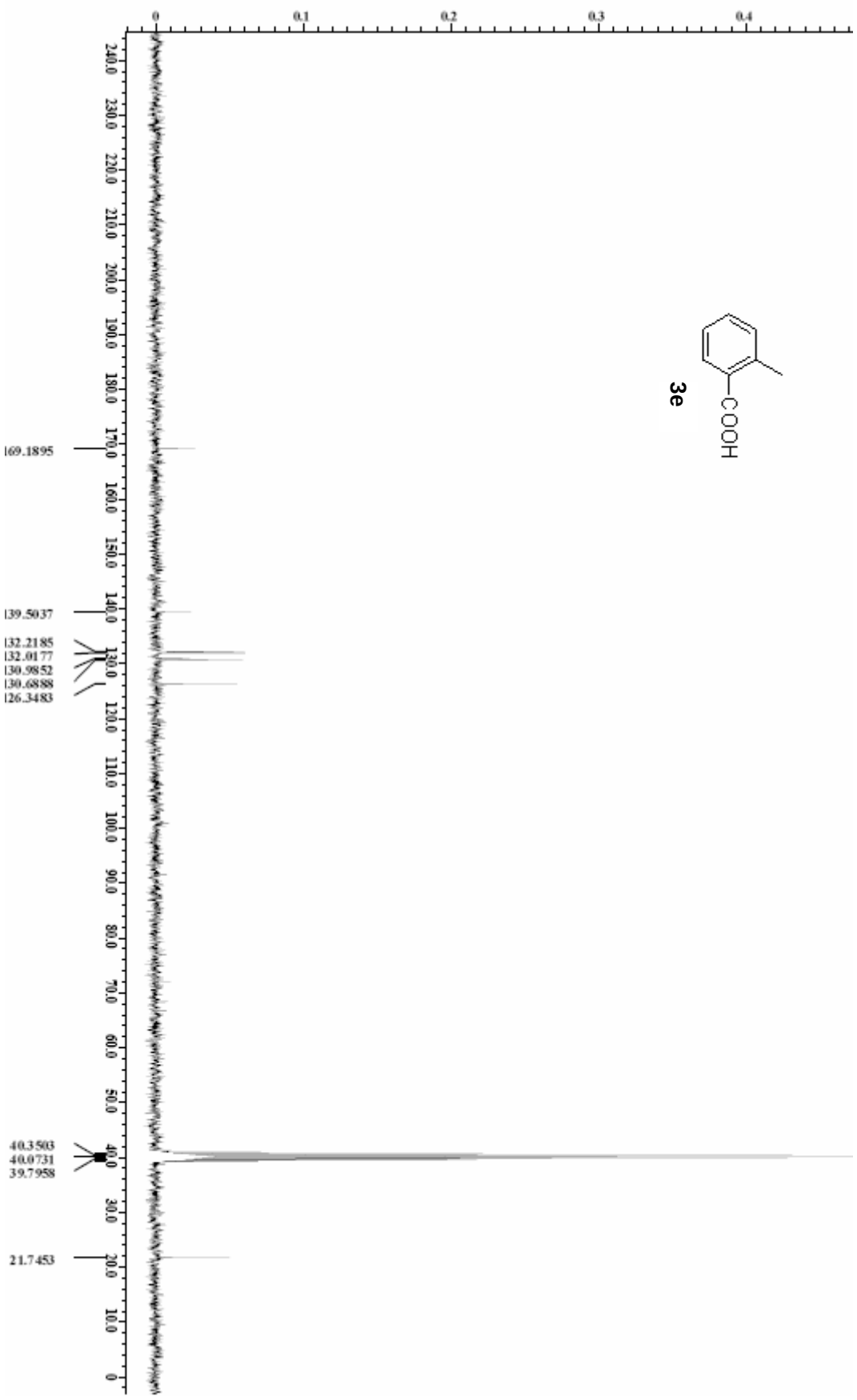
0.946
1
1.055
2.066
3.019
3e
COOH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COOH
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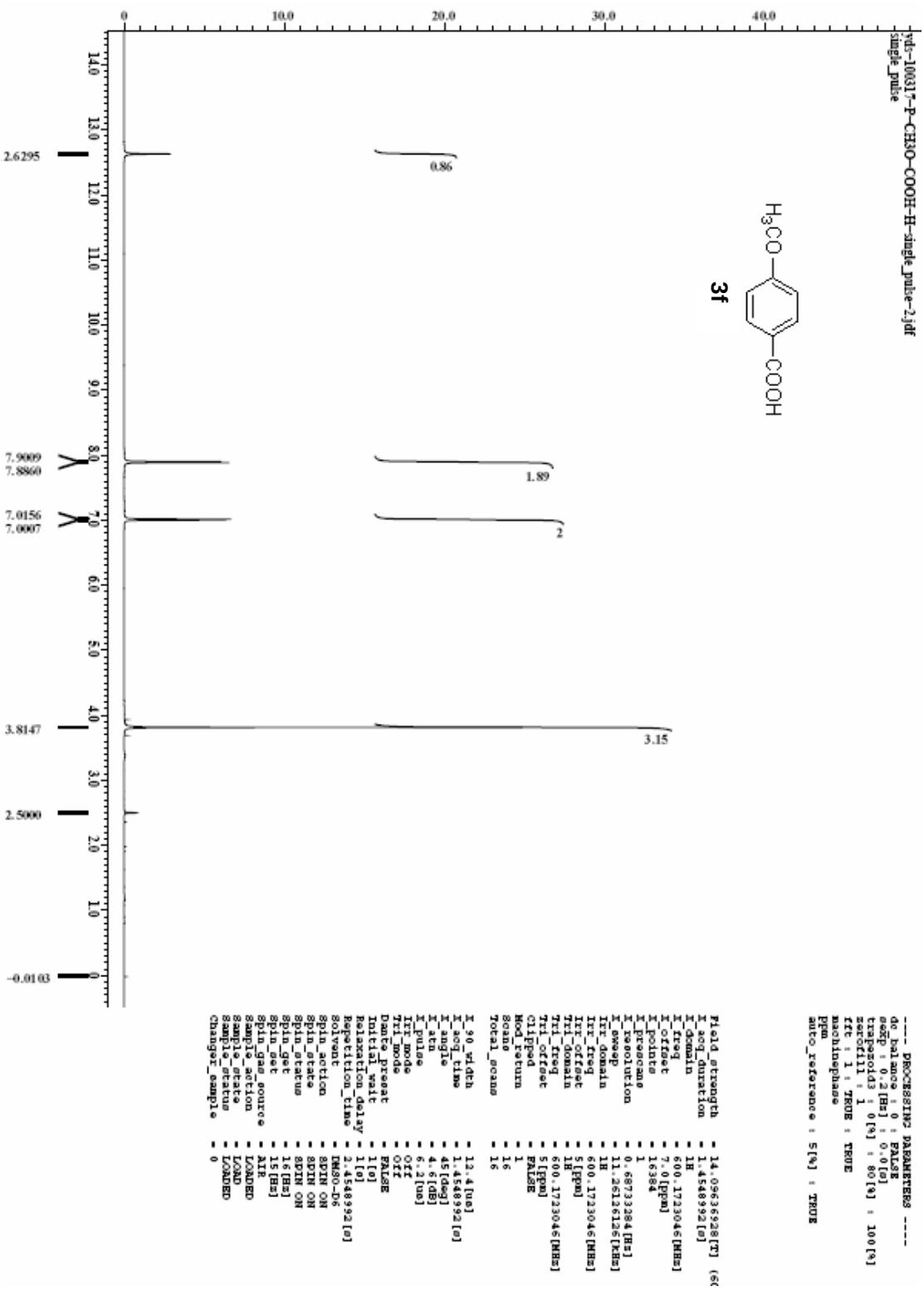
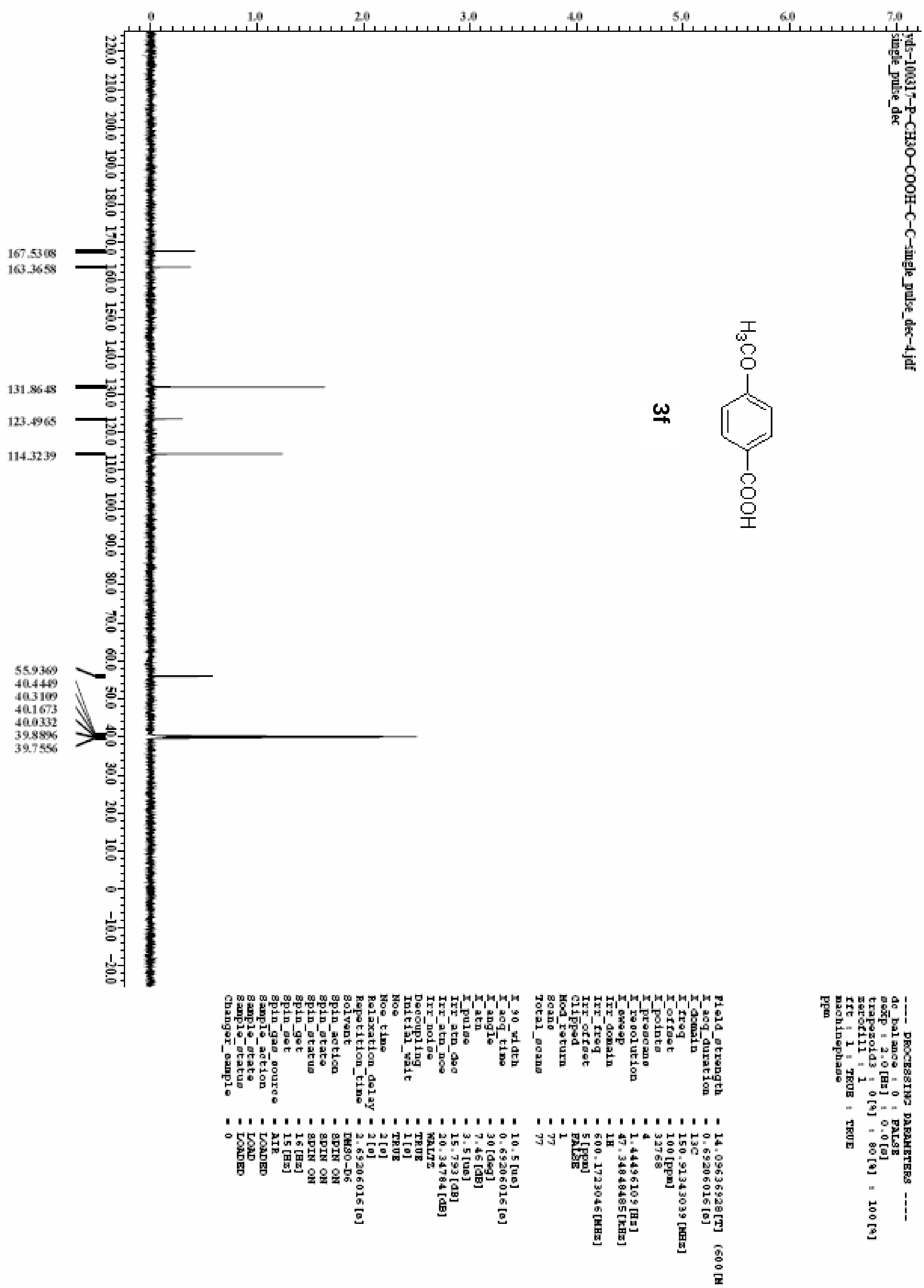
132.0177
130.9852
130.6888
126.3483
40.3503
40.0731
39.7958
21.7453


vds-100317-P-CH3O-COOH-H-single_pulse-1.jdf
single_pulse
H3CO
COOH
3f
2.6295
7.9009
7.8860
7.0156
7.0007
3.8147
2.5000
-0.0103
0.86
1.89
3.15
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
dcOp_axis : 0[Hz] : 0.0[s]
trapezoid : 1.0[s] : 80[%] : 100[%]
zerofill : 1 : TRUE : TRUE
frt : 1 : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE
Field_strength - 14.09636928[T] (6
X_acq_duration - 1.4548992[s]
X_domain - 1H
X_freq - 600.1723046[MHz]
X_offset - 7.0[ppm]
X_points - 16384
X_prescans - 1
X_resolution - 0.68733384[Hz]
X_sweep - 11.2612126[kHz]
Irr_domain - 1H
Irr_freq - 600.1723046[MHz]
Irr_offset - 5[ppm]
Irr_domain - 1H
Irr_freq - 600.1723046[MHz]
Tri_offset - 5[ppm]
Clipped - FALSE
Mod_return - 1
Scans - 16
Total_scans - 16
X_90_width - 12.4[us]
X_acq_time - 1.4548992[s]
X_angle - 45[deg]
X_atn - 4.6[dB]
X_pulse - 6.2[us]
Irr_mode - Off
Tri_mode - Off
Dante_Preset - FALSE
Initial_wait - 1[s]
Relaxation_delay - 1[s]
Repetition_time - 2.4548992[s]
Solvent - DMSO-D6
Spin_action - SPIN ON
Spin_state - SPIN ON
Spin_status - SPIN ON
Spin_set - 16[Hz]
Spin_gas_source - AIR
Sample_action - LOADED
Sample_state - LOAD
Sample_status - LOADED
Changer_sample - 0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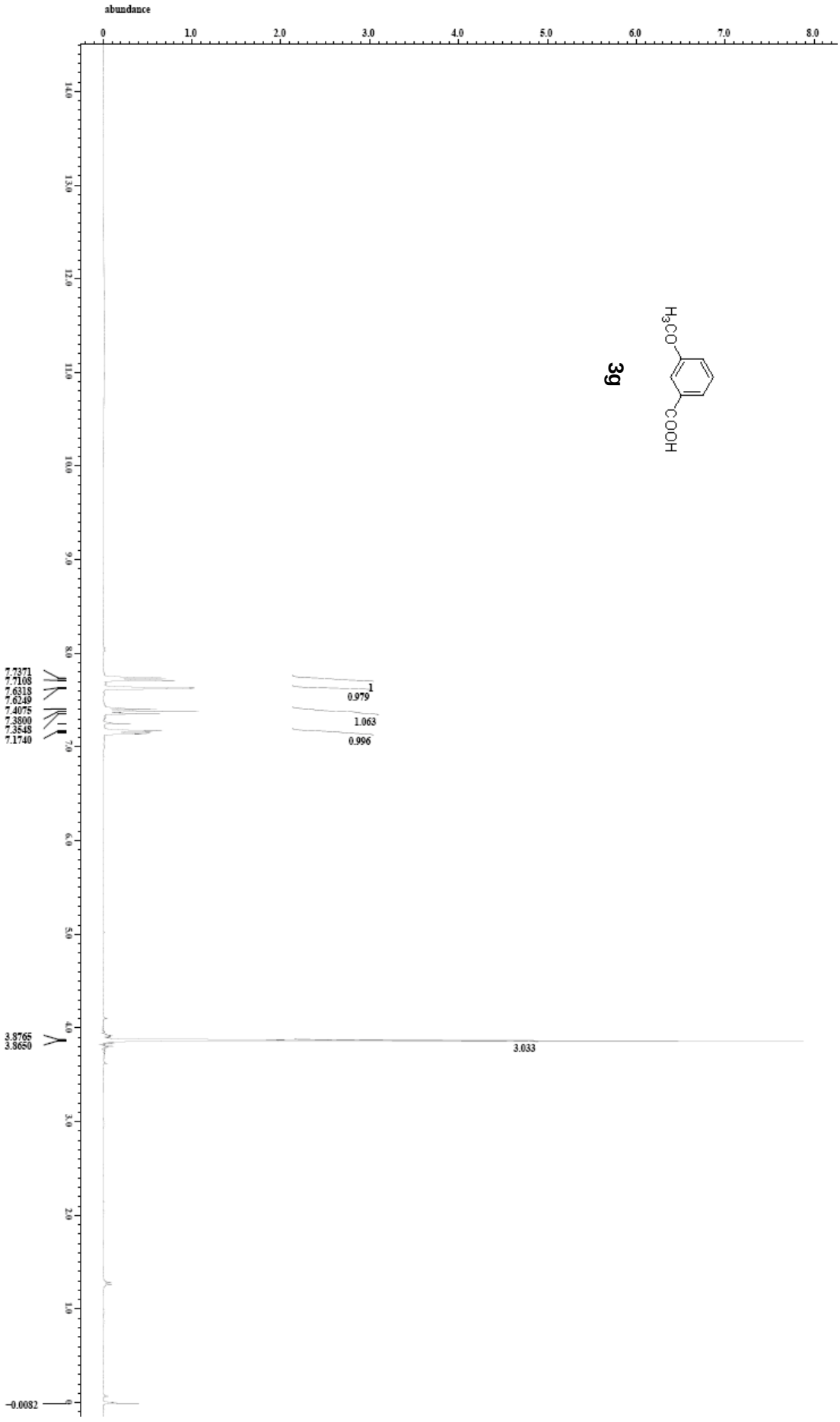
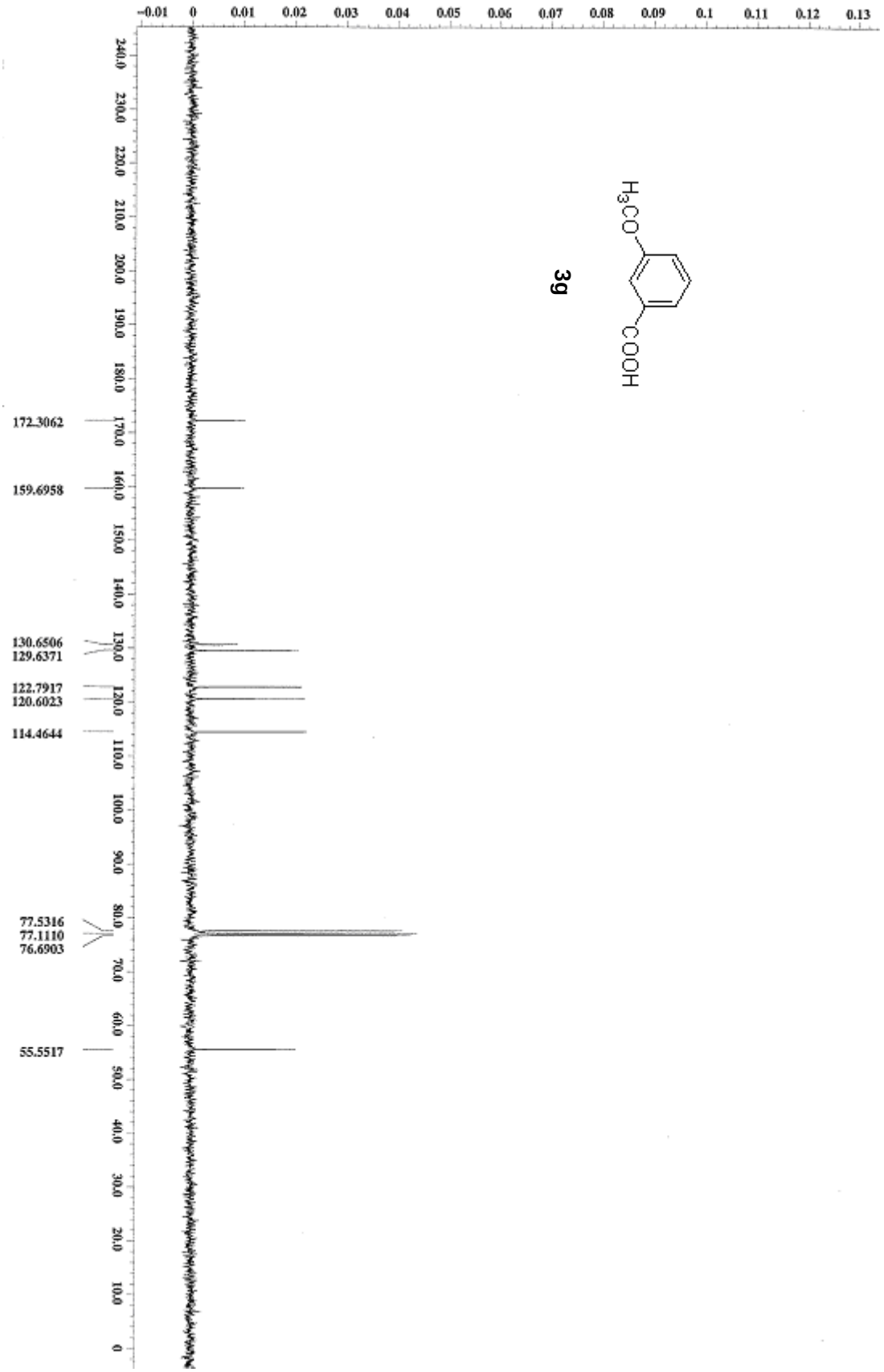
131.8648
123.4965
114.3239
55.9369
40.4449
40.3109
40.1673
40.0332
39.8896
39.7556
3f


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
3g
H3CO
COOH
7.7371
7.7108
7.6318
7.6249
7.4075
7.3800
7.3548
7.1740
1
0.979
1.063
0.996
3.9765
3.8650
3.033
−0.0082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130.6506
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122.7917
120.6023
114.4644
77.5316
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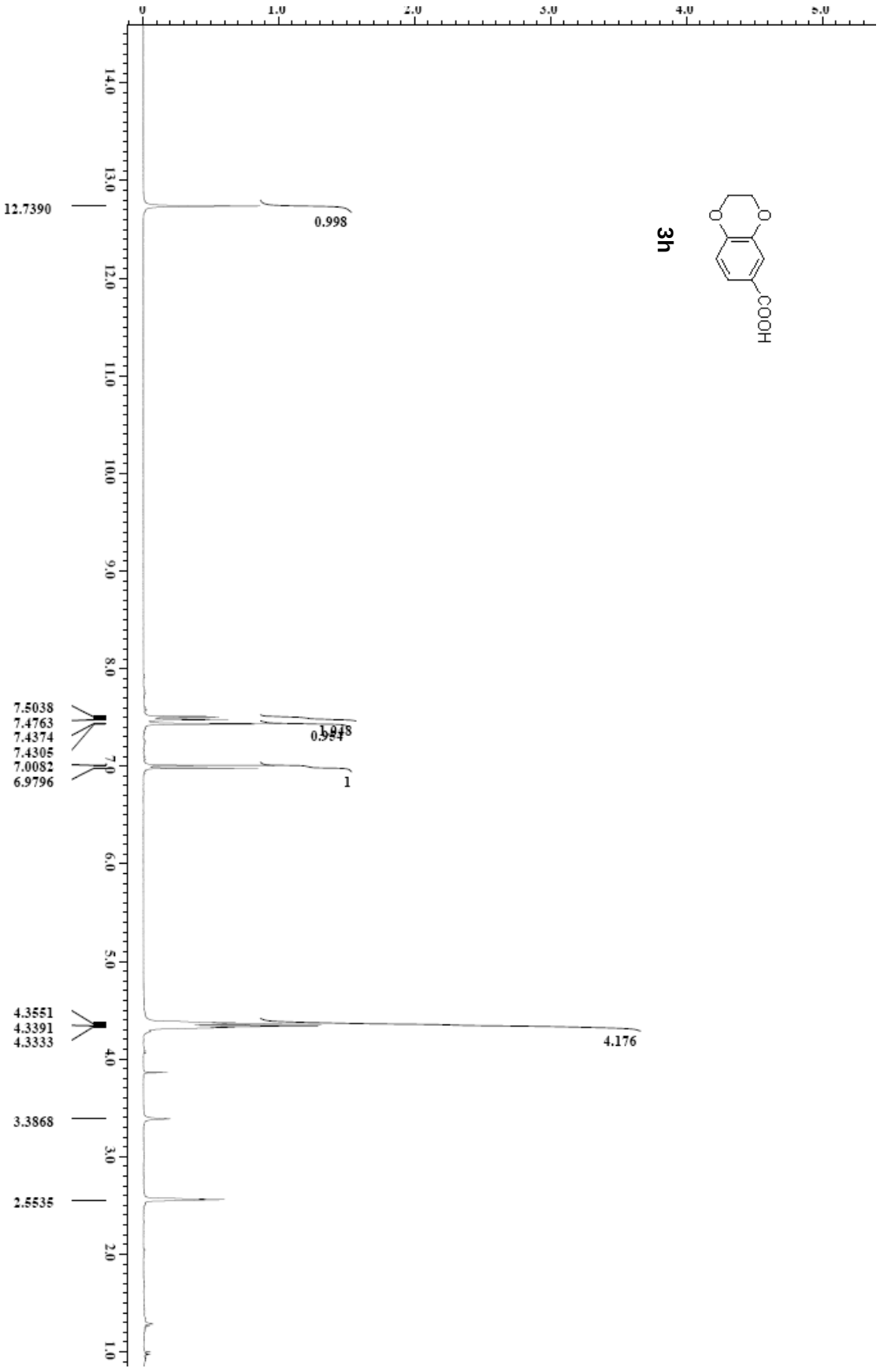
76.6903
55.5517
3g
H3CO
COOH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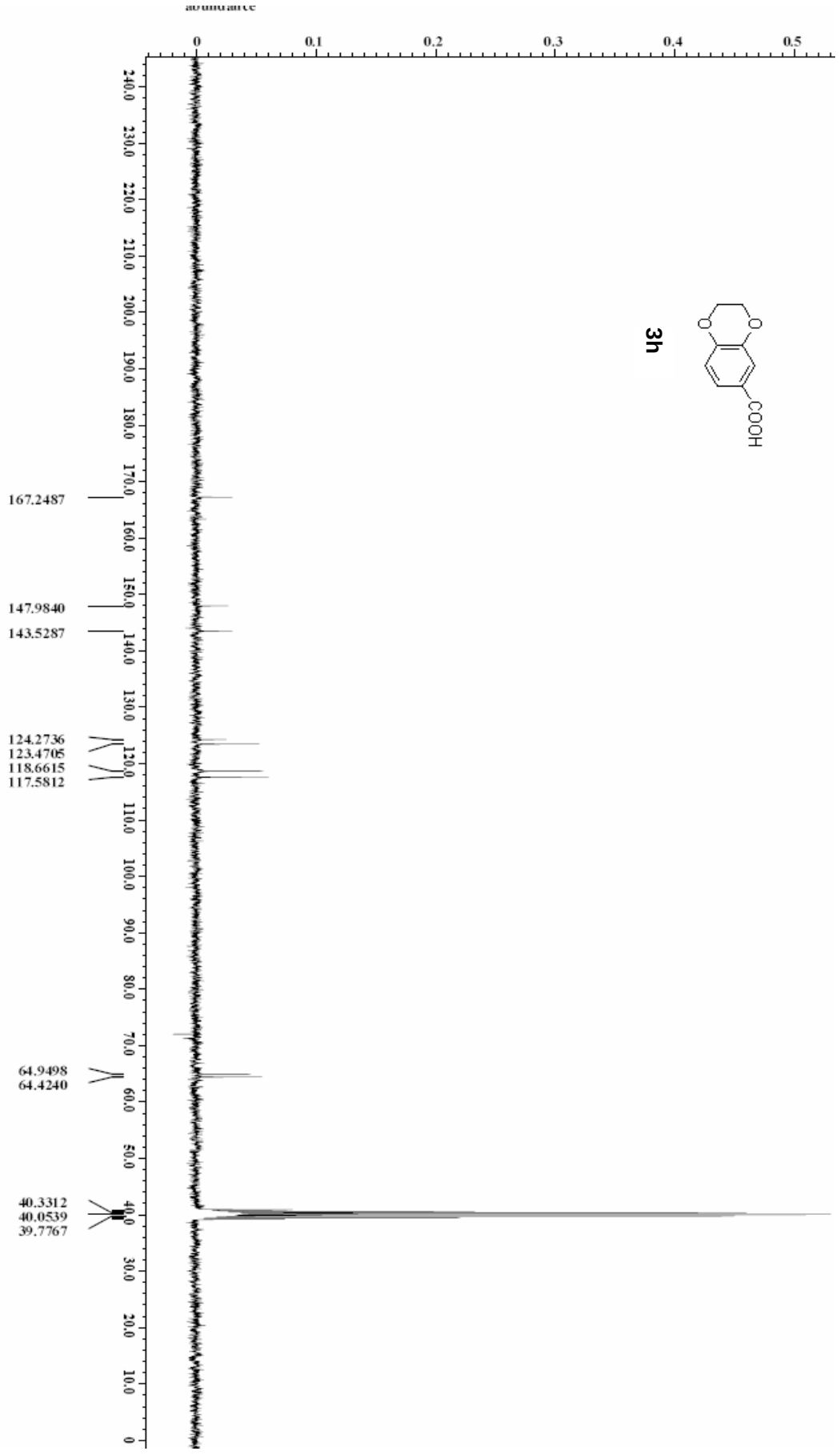
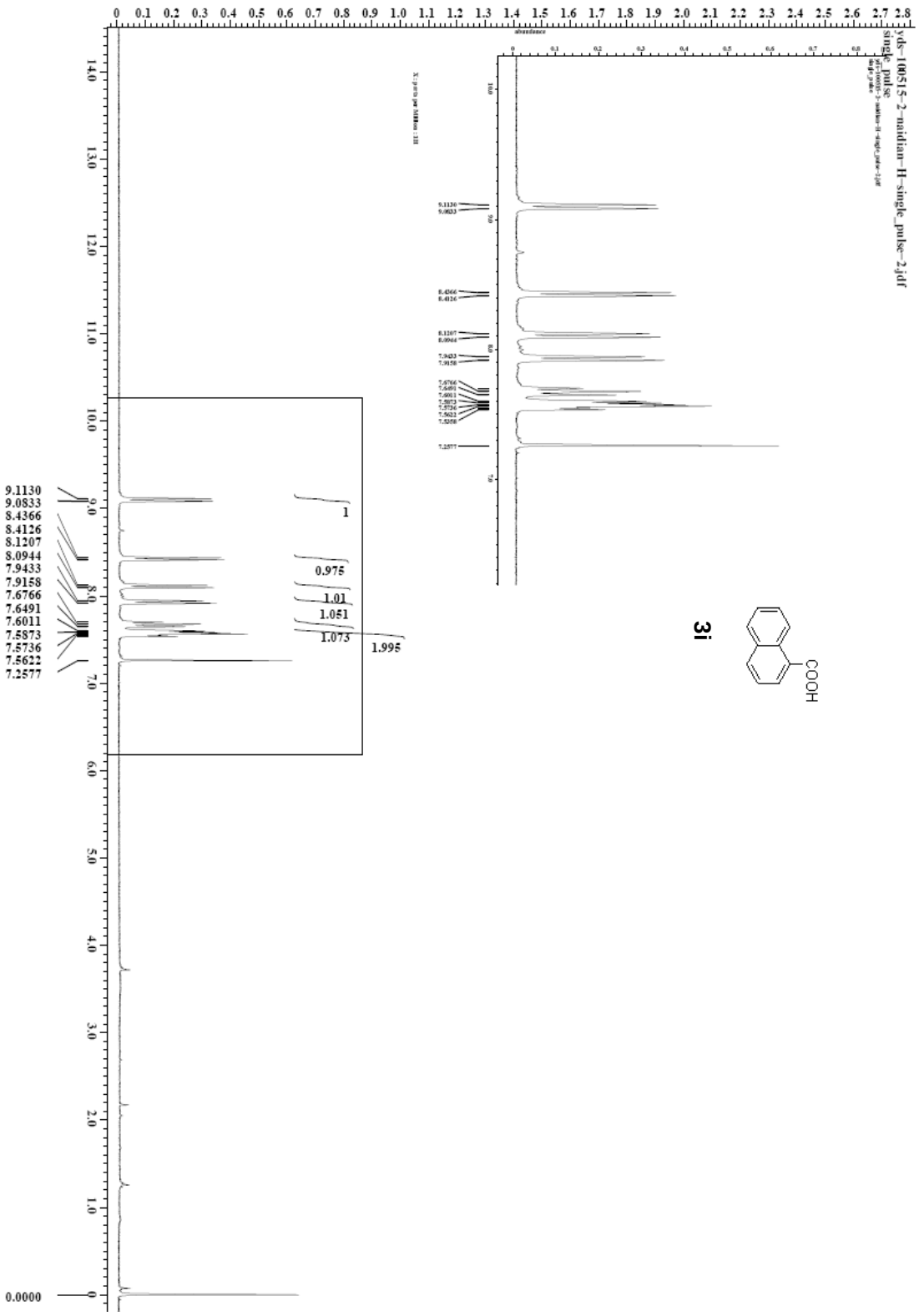
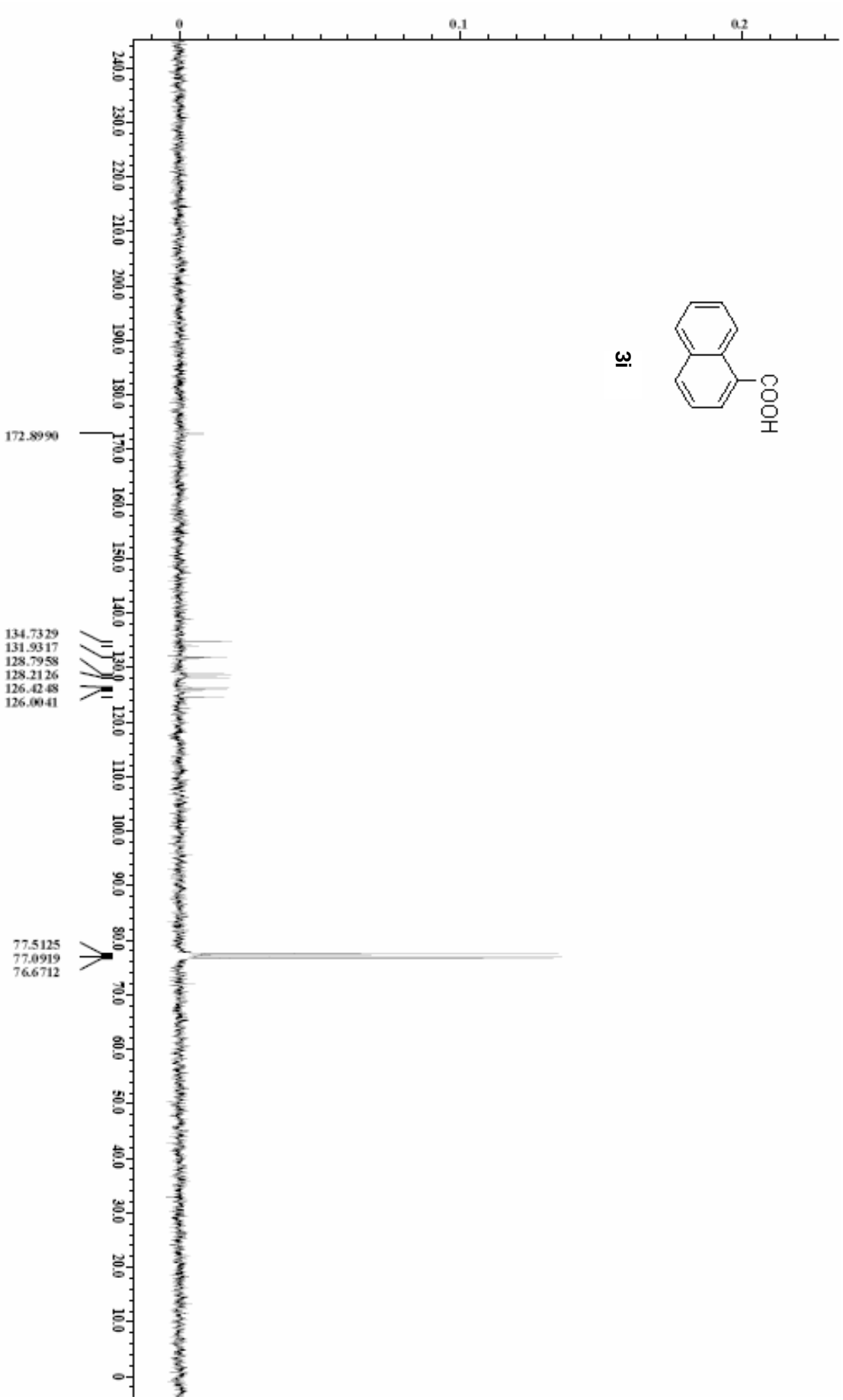
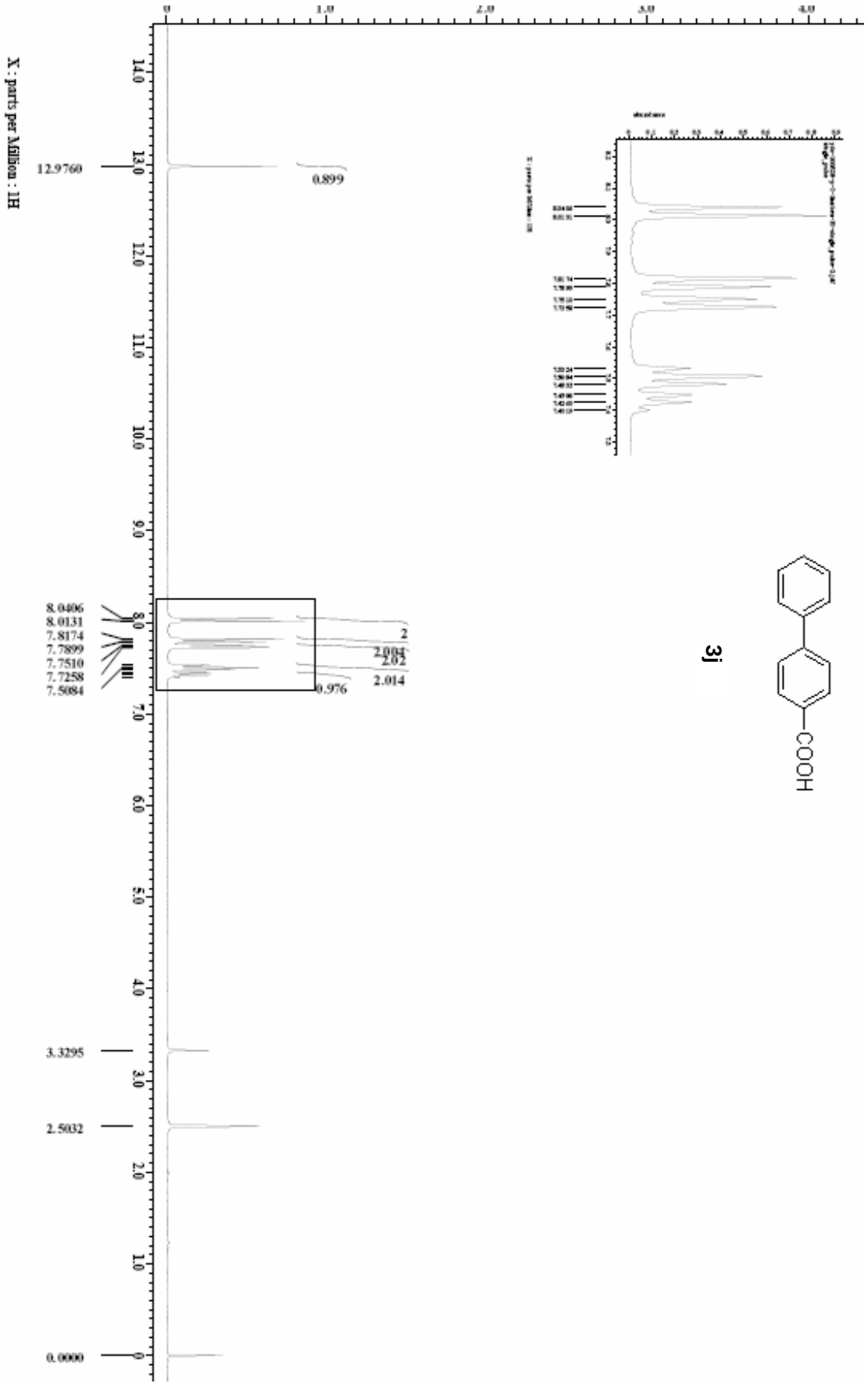
0.998
7.5038
7.4763
7.4374
7.4305
7.0082
6.9796
1
4.3551
4.3391
4.3333
4.176
3.3868
2.5535
3h
COOH


abundance
0
0.1
0.2
0.3
0.4
0.5
3h
COOH
167.2487
147.9840
143.5287
124.2736
123.4705
118.6615
117.5812
64.9498
64.4240
40.3312
40.0539
39.7767


xdc-100515-2-naidian-H-single_pulse-2.jdf
single_pulse
9.1130
9.0833
8.4366
8.4126
8.1207
8.0944
7.9433
7.9158
7.6766
7.6491
7.6011
7.5873
7.5736
7.5622
7.2577
0.0000
1
0.975
1.01
1.051
1.073
1.995
3i
COOH


0
0.1
0.2
240.0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
172.8990
134.7329
131.9317
128.7958
128.2126
126.4248
126.0041
77.5125
77.0919
76.6712
3i
COOH


X : parts per Million : 1H
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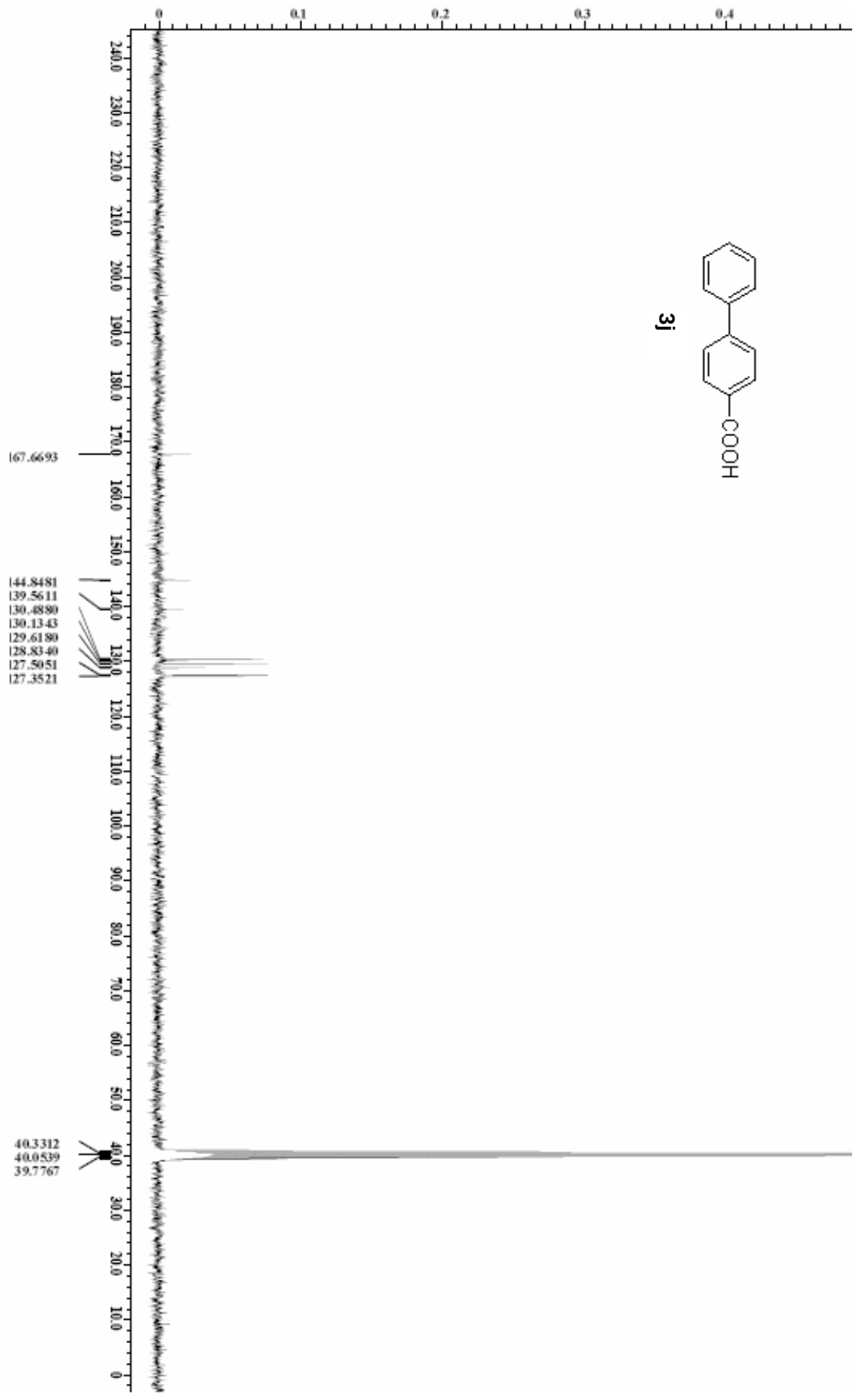
0.899
8.0406
8.0131
7.8174
7.7899
7.7510
7.7258
7.5084
2
2.004
2.02
2.014
0.976
3.3295
2.5032
0.0000
3j
COOH


0
0.1
0.2
0.3
0.4
240.0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.6693
144.8481
139.5611
130.4880
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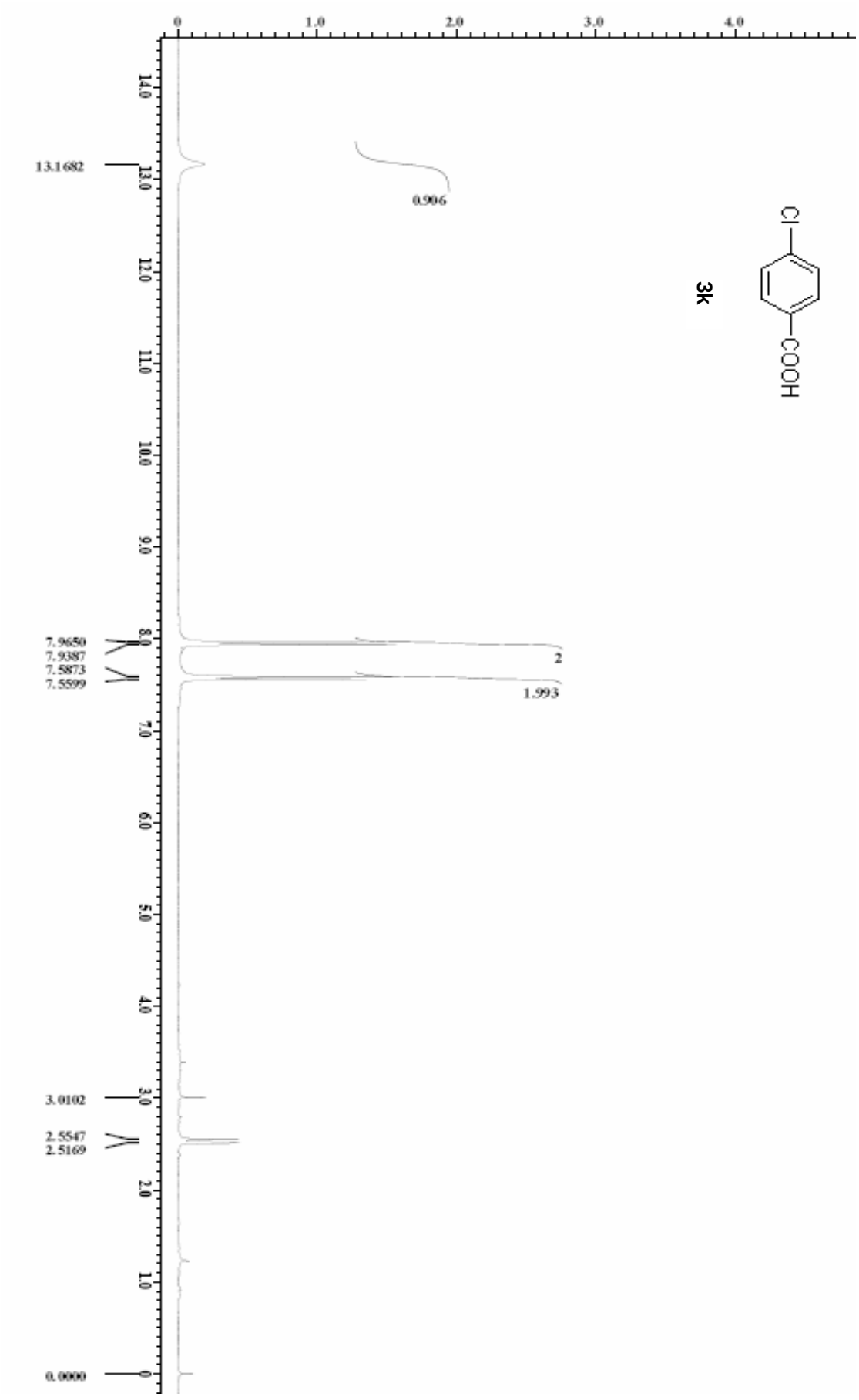
128.8340
127.5051
127.3521
40.3312
40.0539
39.7767
3i
COOH


0
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2.0
3.0
4.0
13.1682
0.906
3k
Cl
COOH
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7.5599
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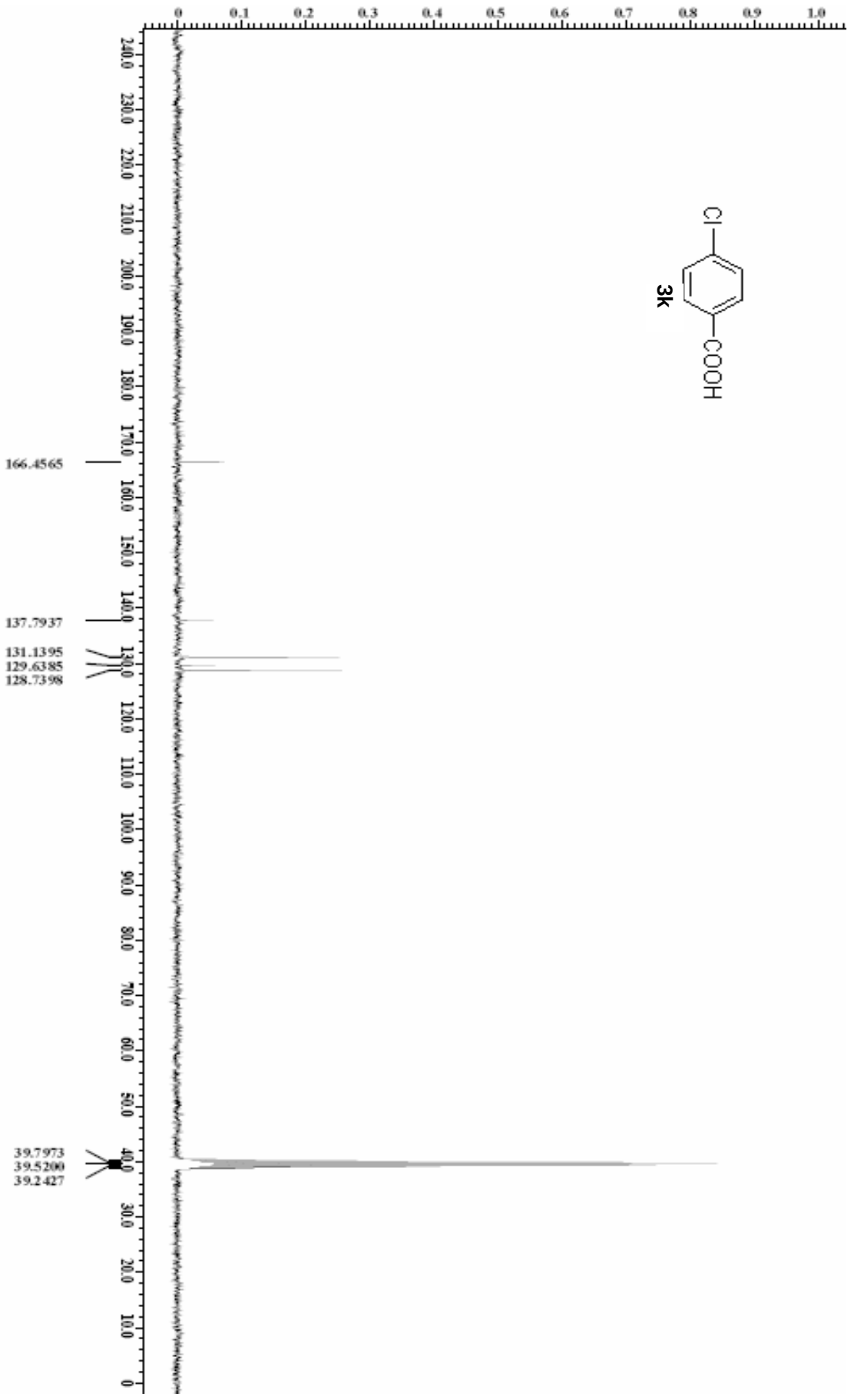
2.5169
0.0000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39.5200
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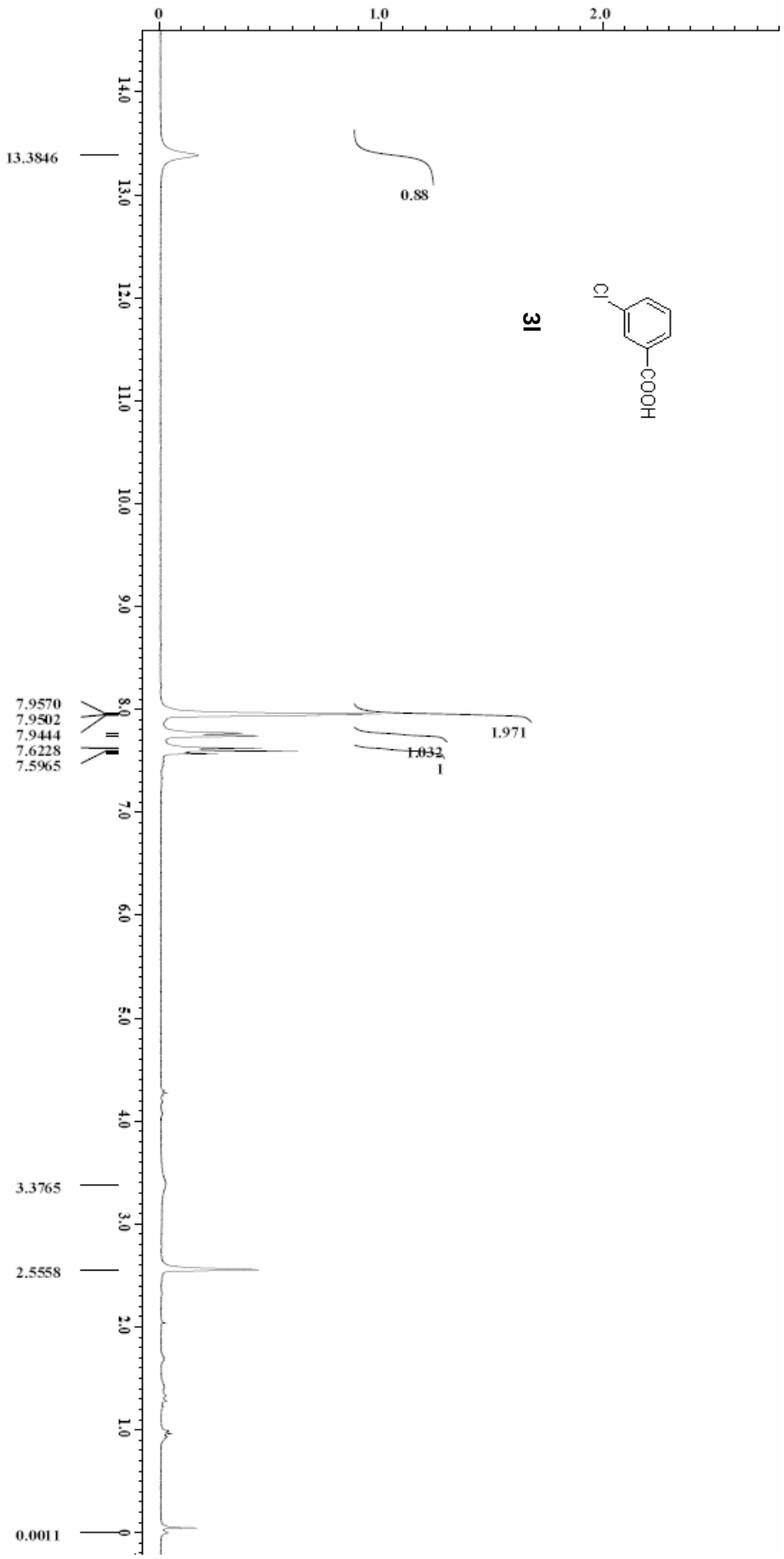
3k
Cl
COOH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7.9444
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3.3765
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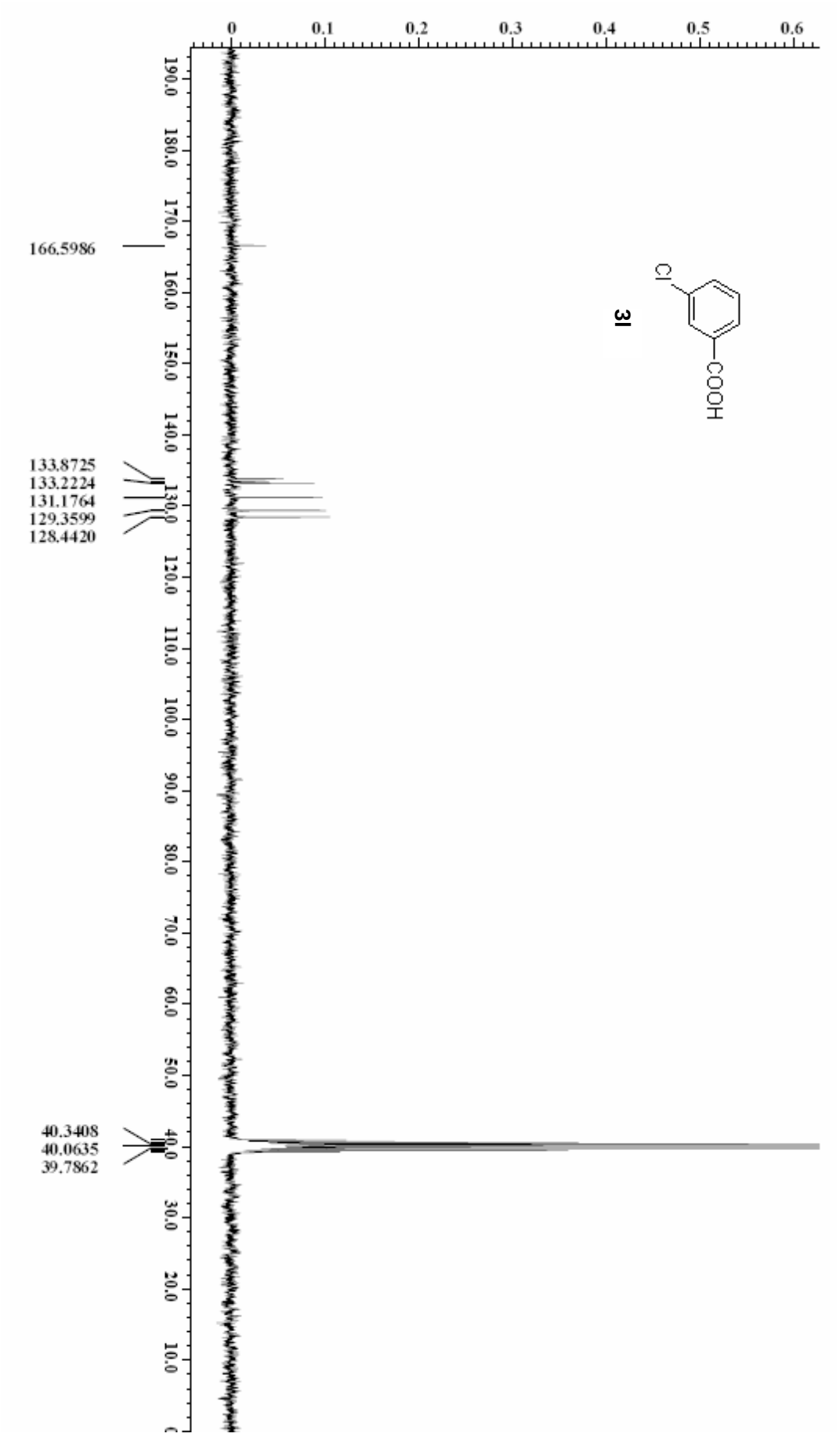
1.032
1
3l
Cl
COOH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131.1764
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128.4420
40.3408
40.0635
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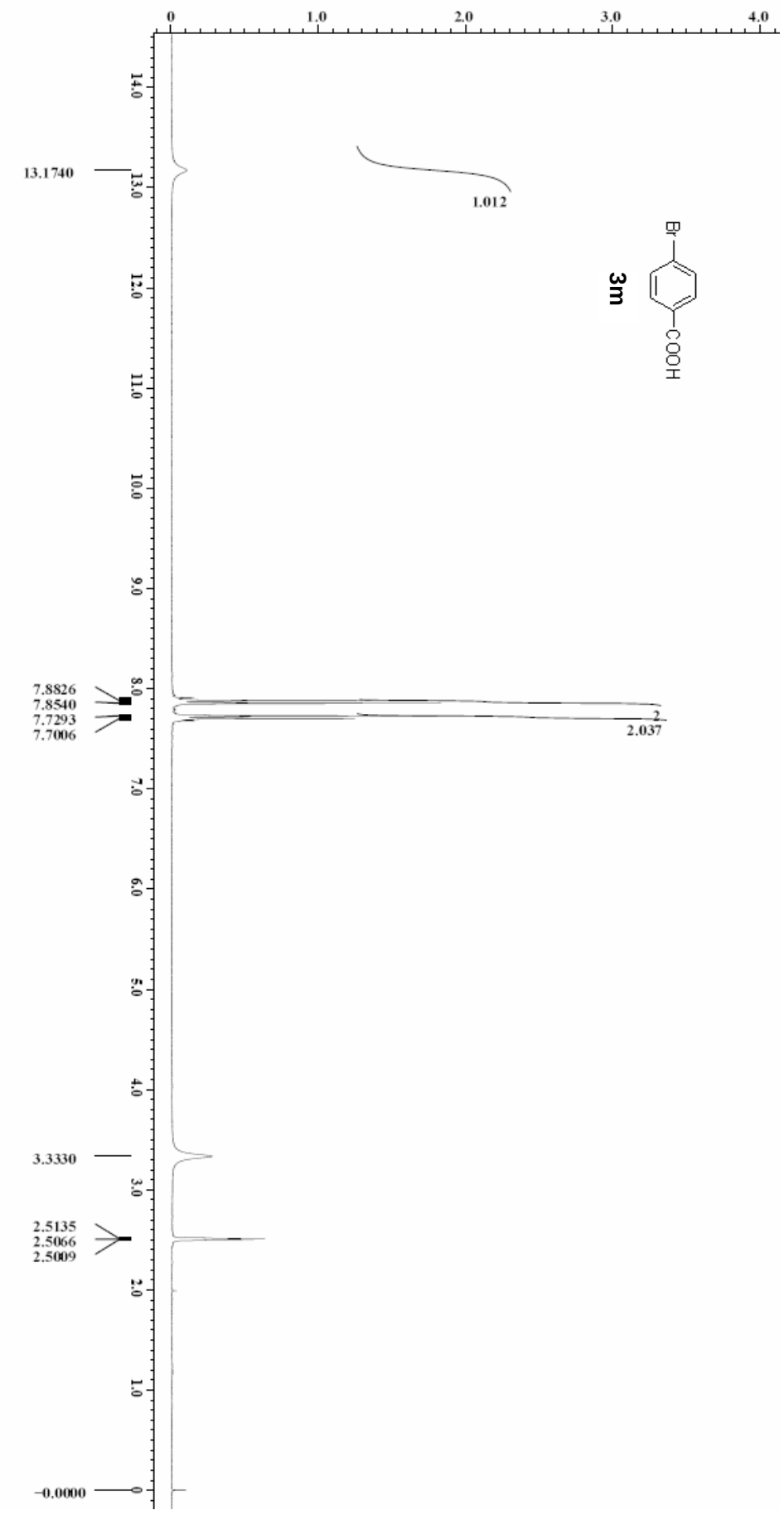
COOH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7.8826
7.8540
7.7293
7.7006
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2.5135
2.5066
2.5009
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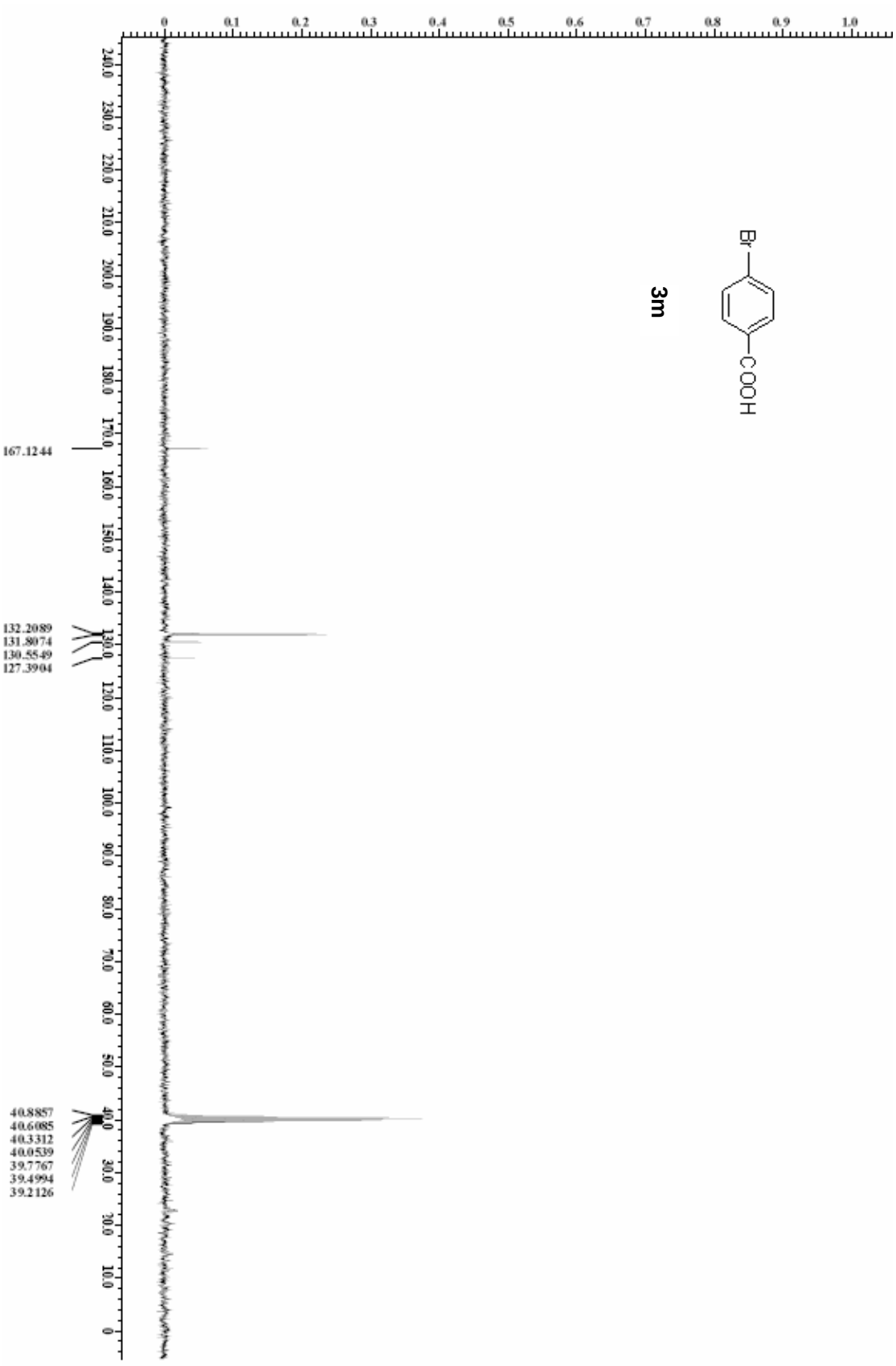
1.012
2.037
3m
Br
COOH


3m
Br
COOH
167.1244
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127.3904
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40.6085
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40.0539
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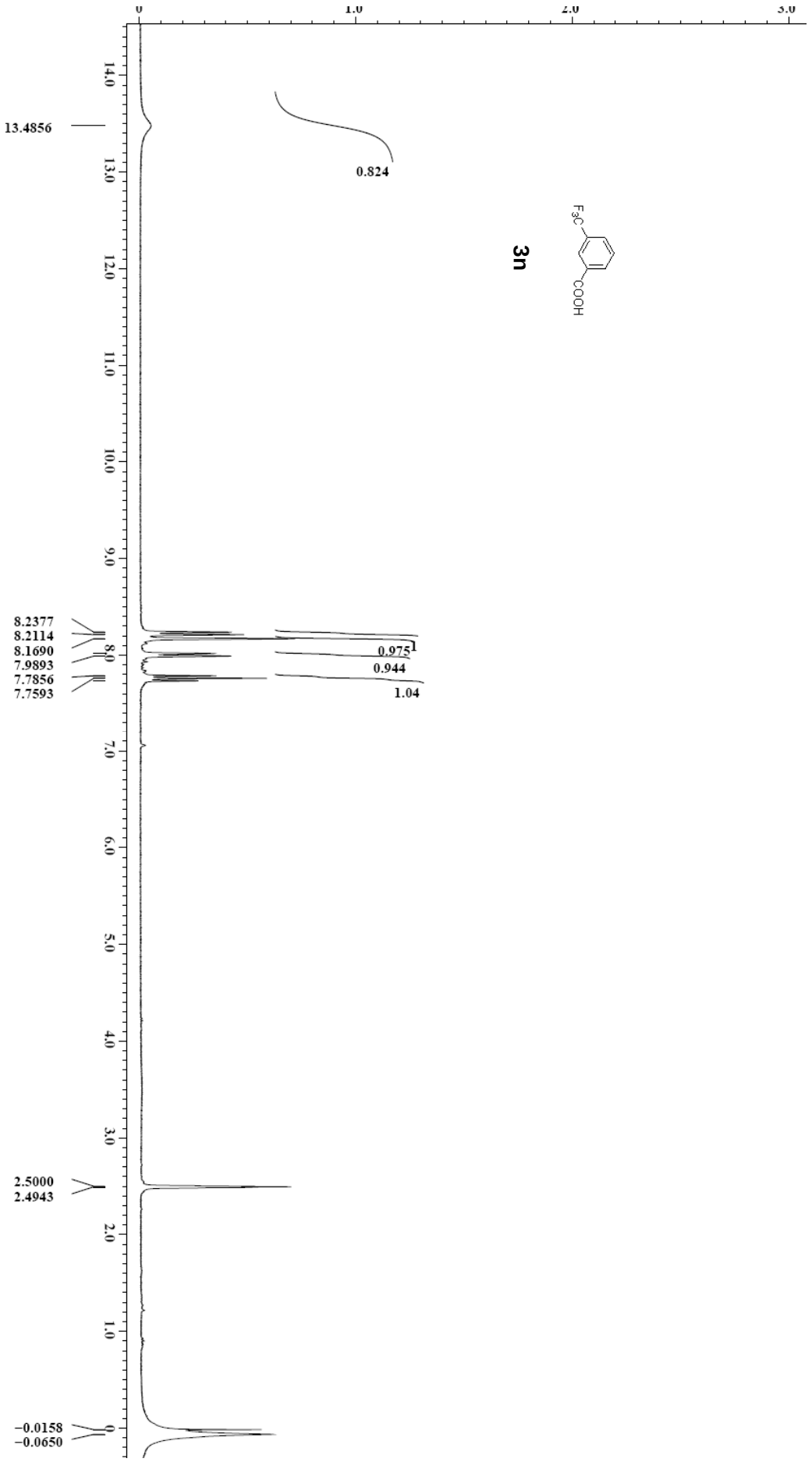
39.2126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7.7856
7.7593
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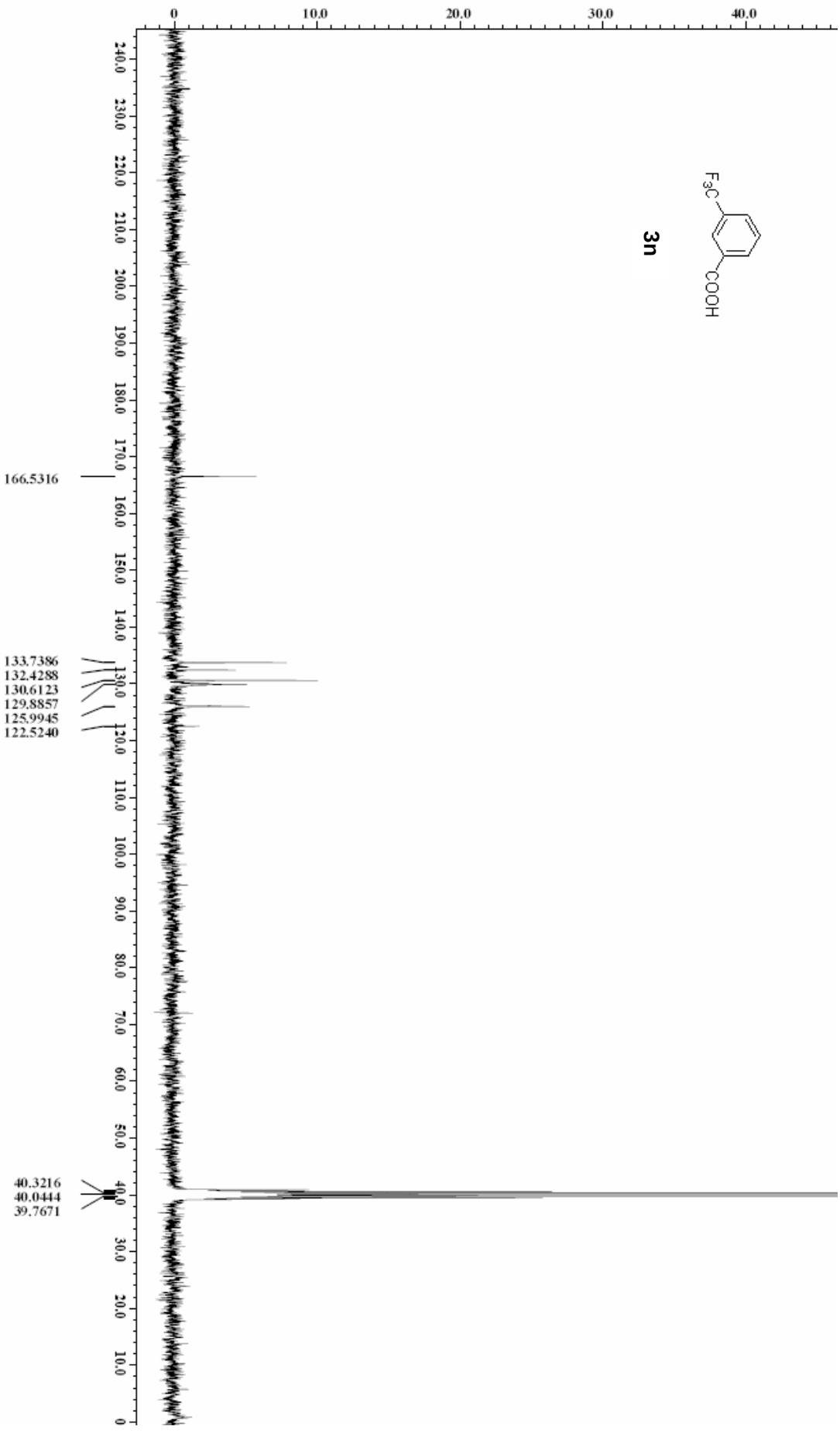
2.4943
−0.0158
−0.0650
0.824
0.975
0.944
1.04
3n
F3C
COOH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133.7386
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130.6123
129.8857
125.9945
122.5240
40.3216
40.0444
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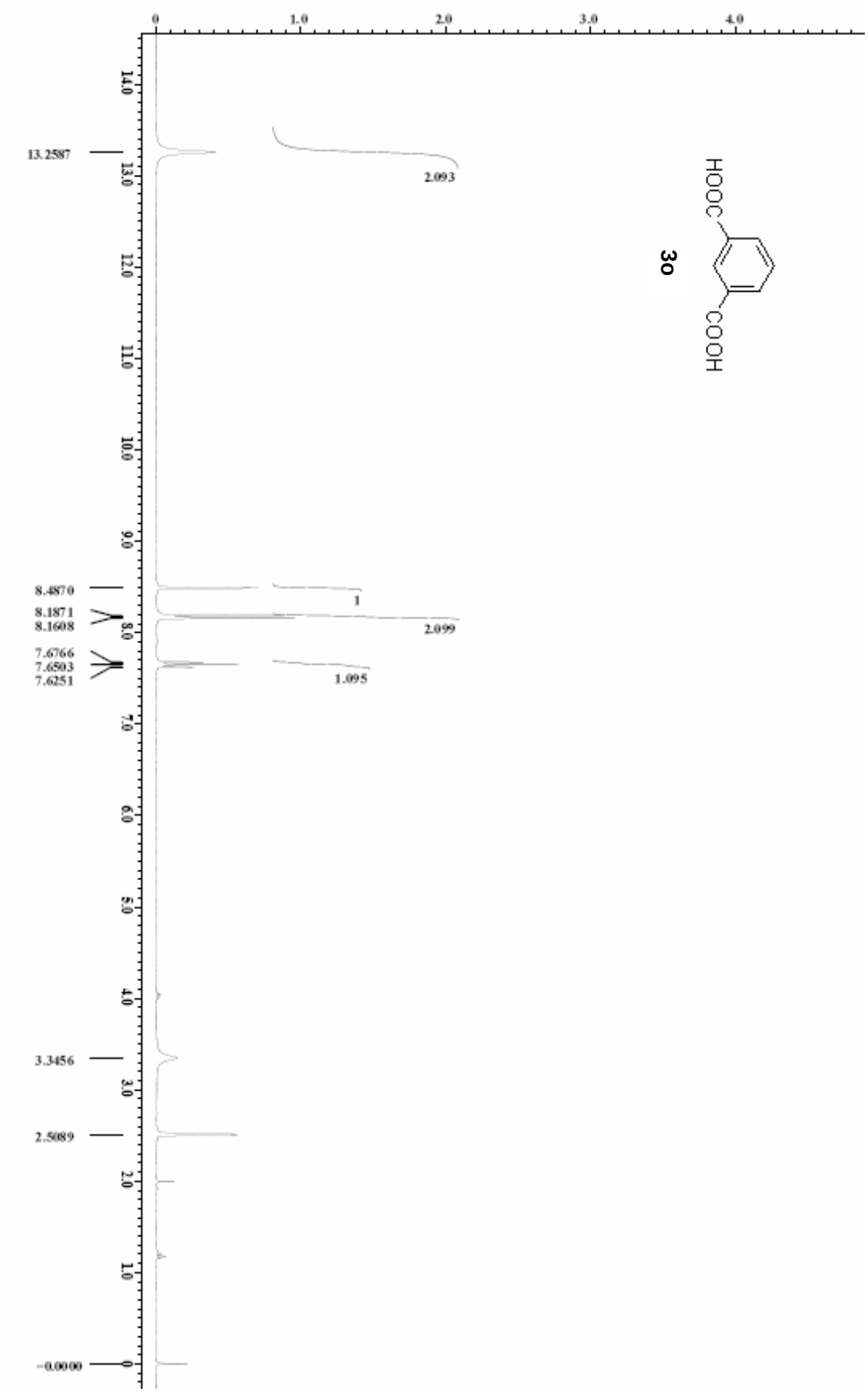
3n
F3C
COOH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8.1871
8.1608
7.6766
7.6503
7.6251
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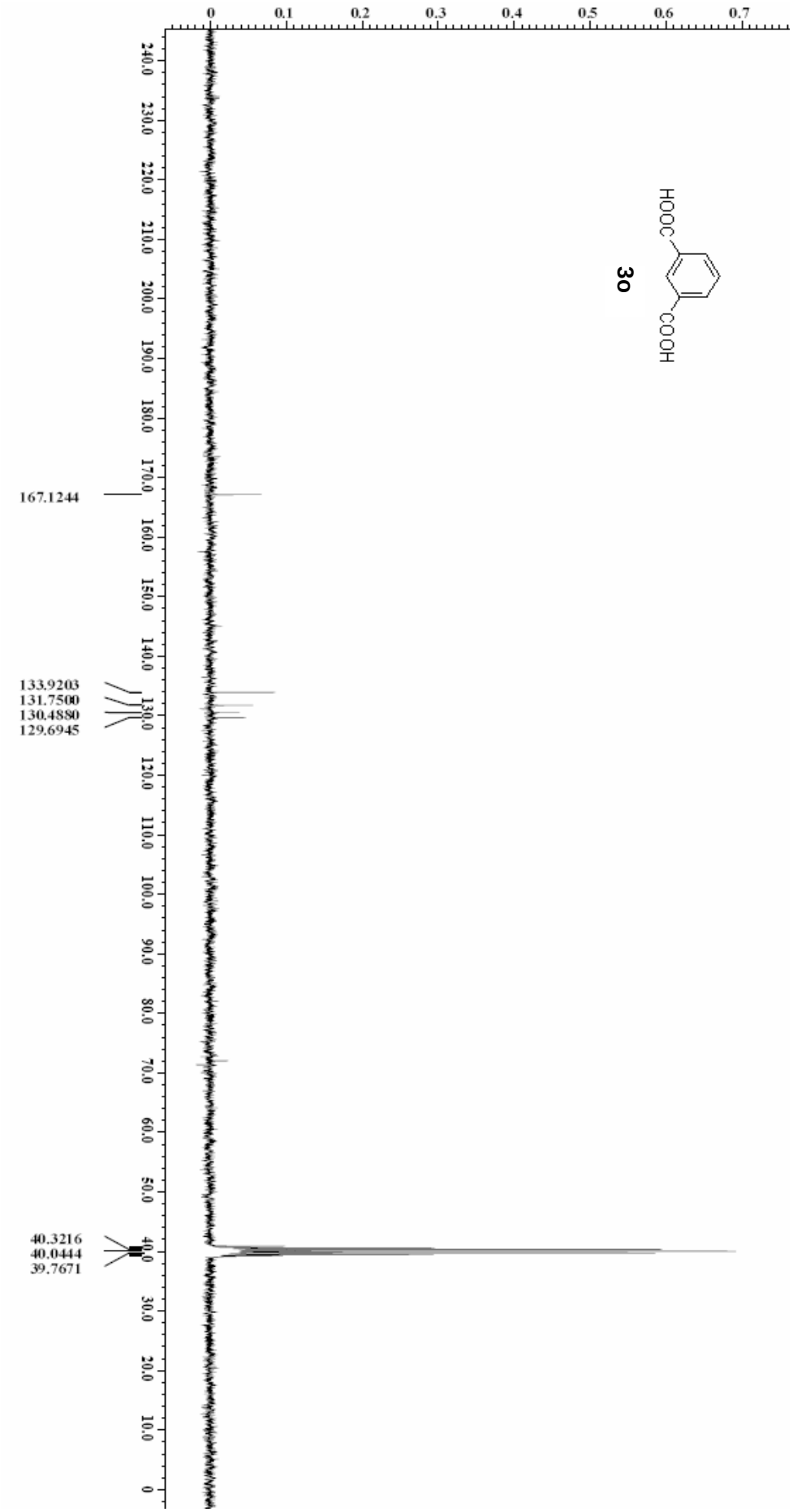
2.093
1
2.099
1.095
HOOC
COOH
3o


HOOC
COOH
3o
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131.7500
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129.6945
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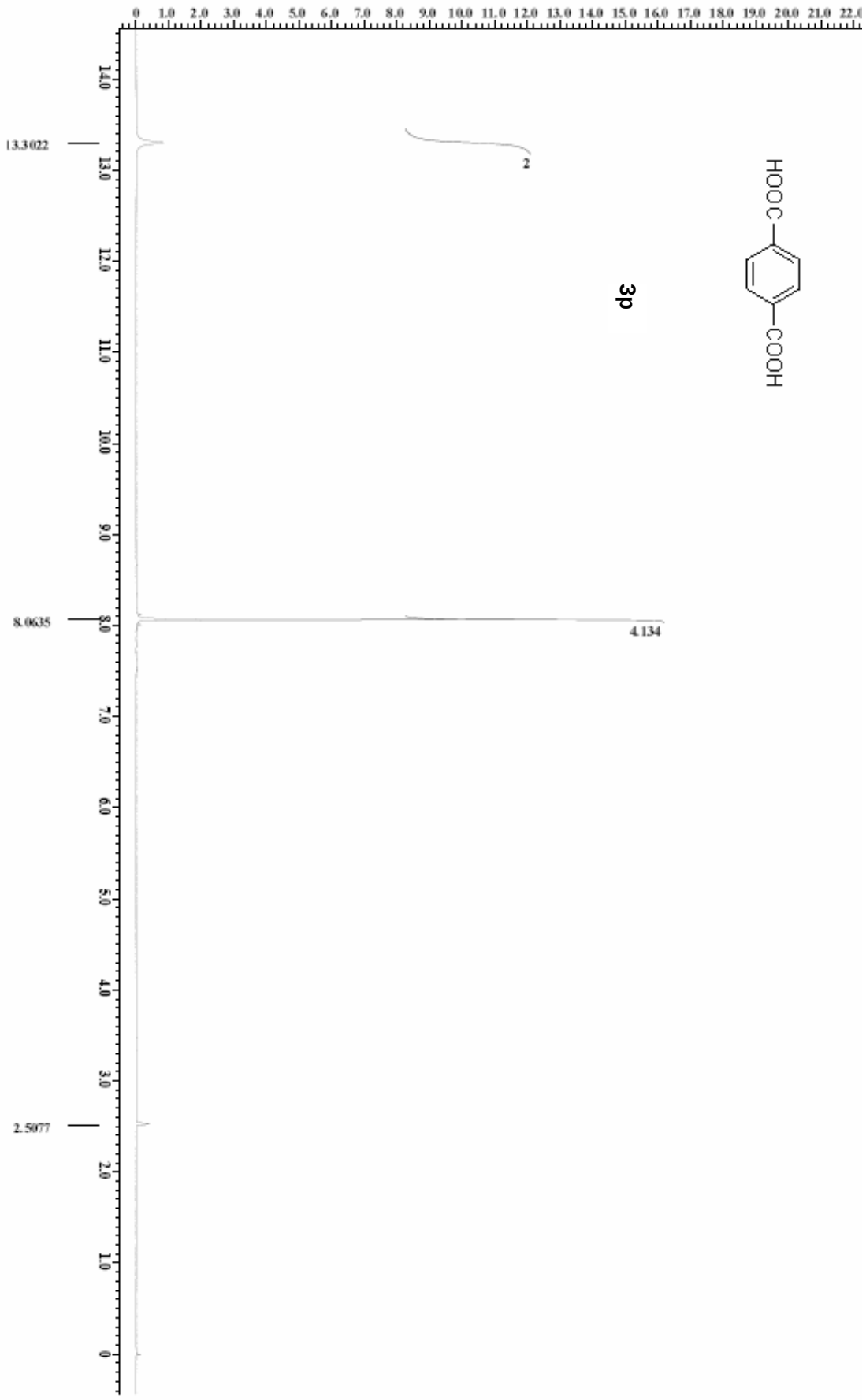
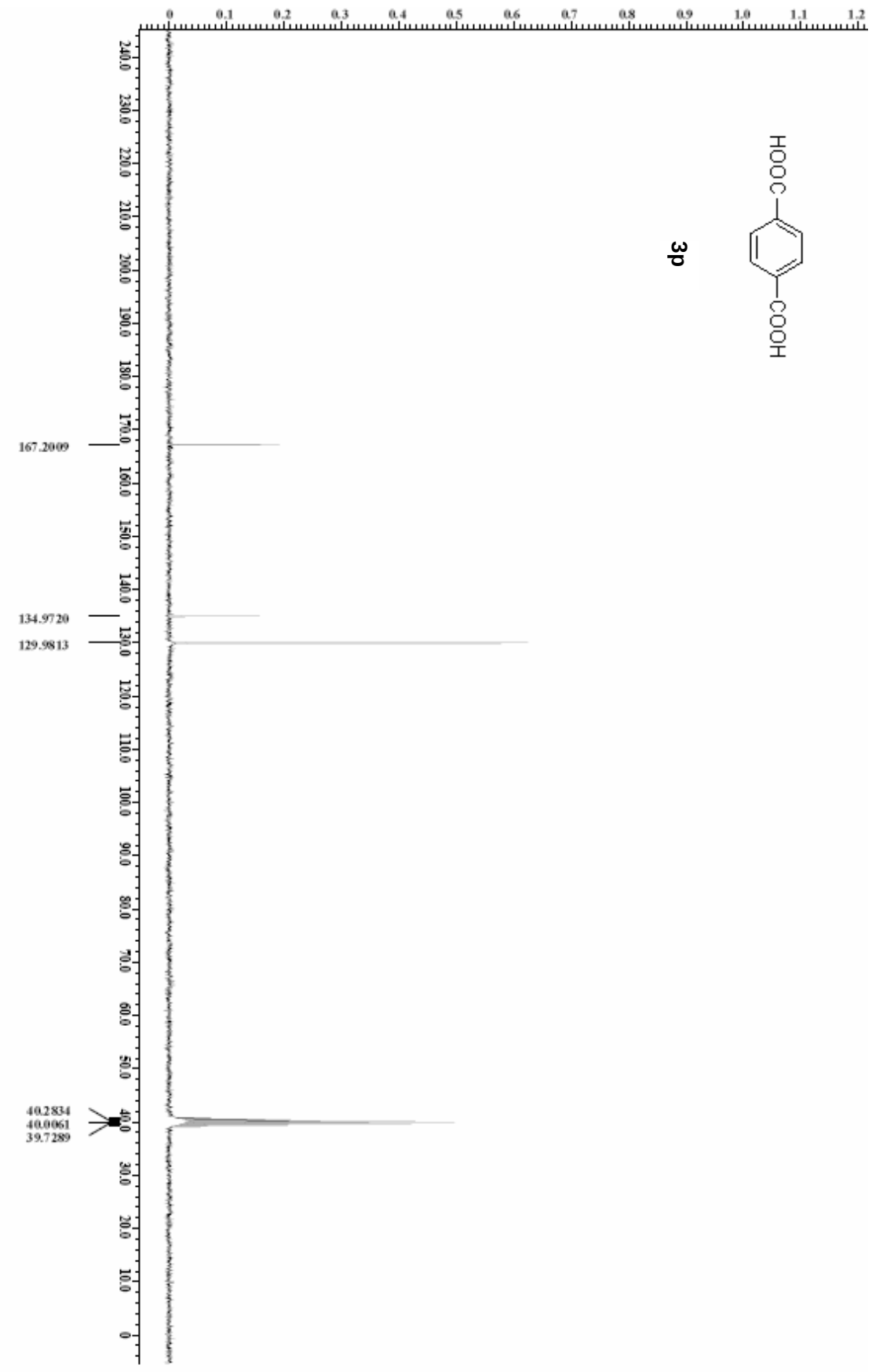
40.0444
39.7671


13.3022
8.0635
2.5077
2
4.134
3p
HOOC
COOH


3p
HOOC
COOH
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129.9813
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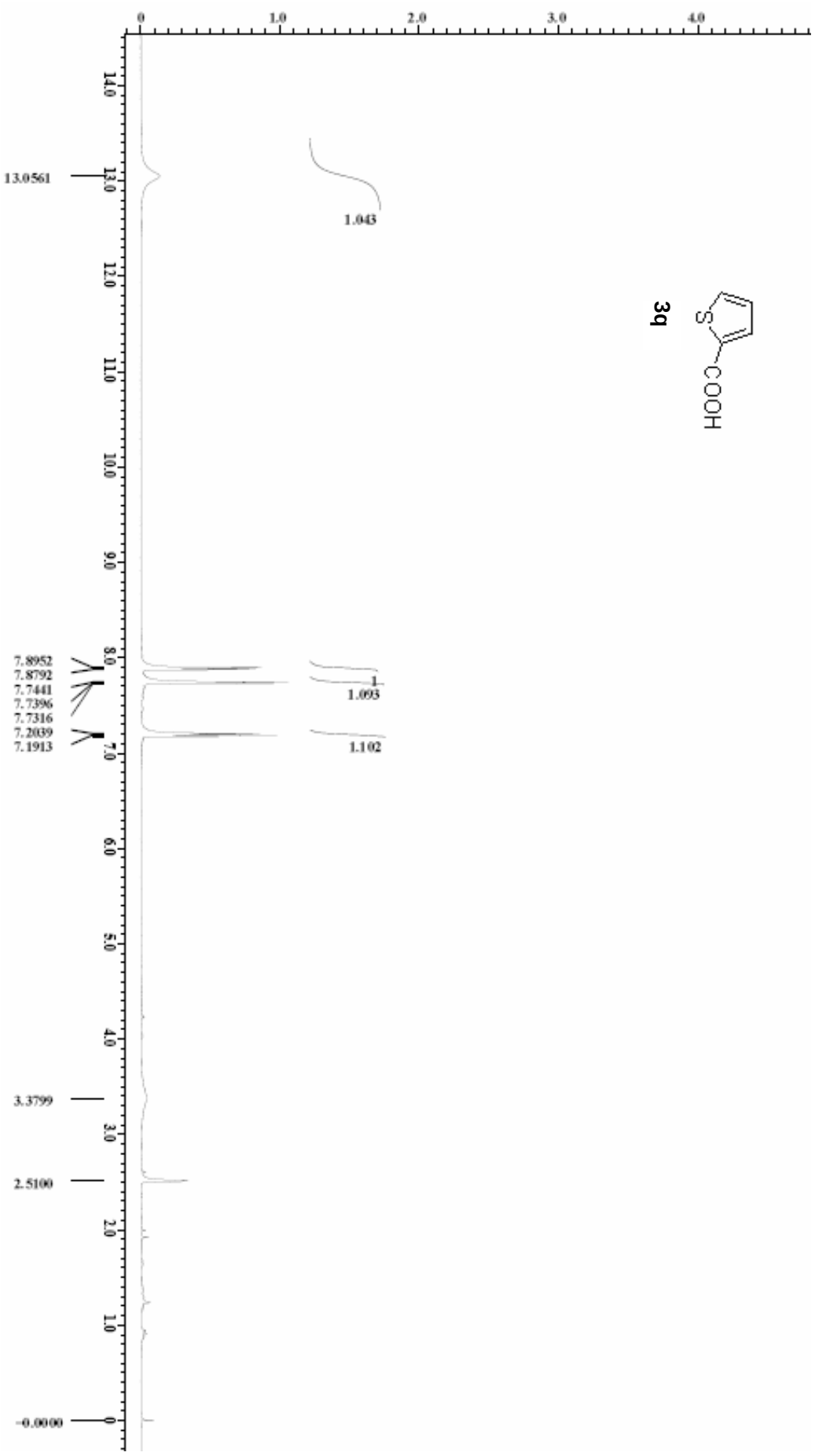
13.0561
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7.8792
7.7441
7.7396
7.7316
7.2039
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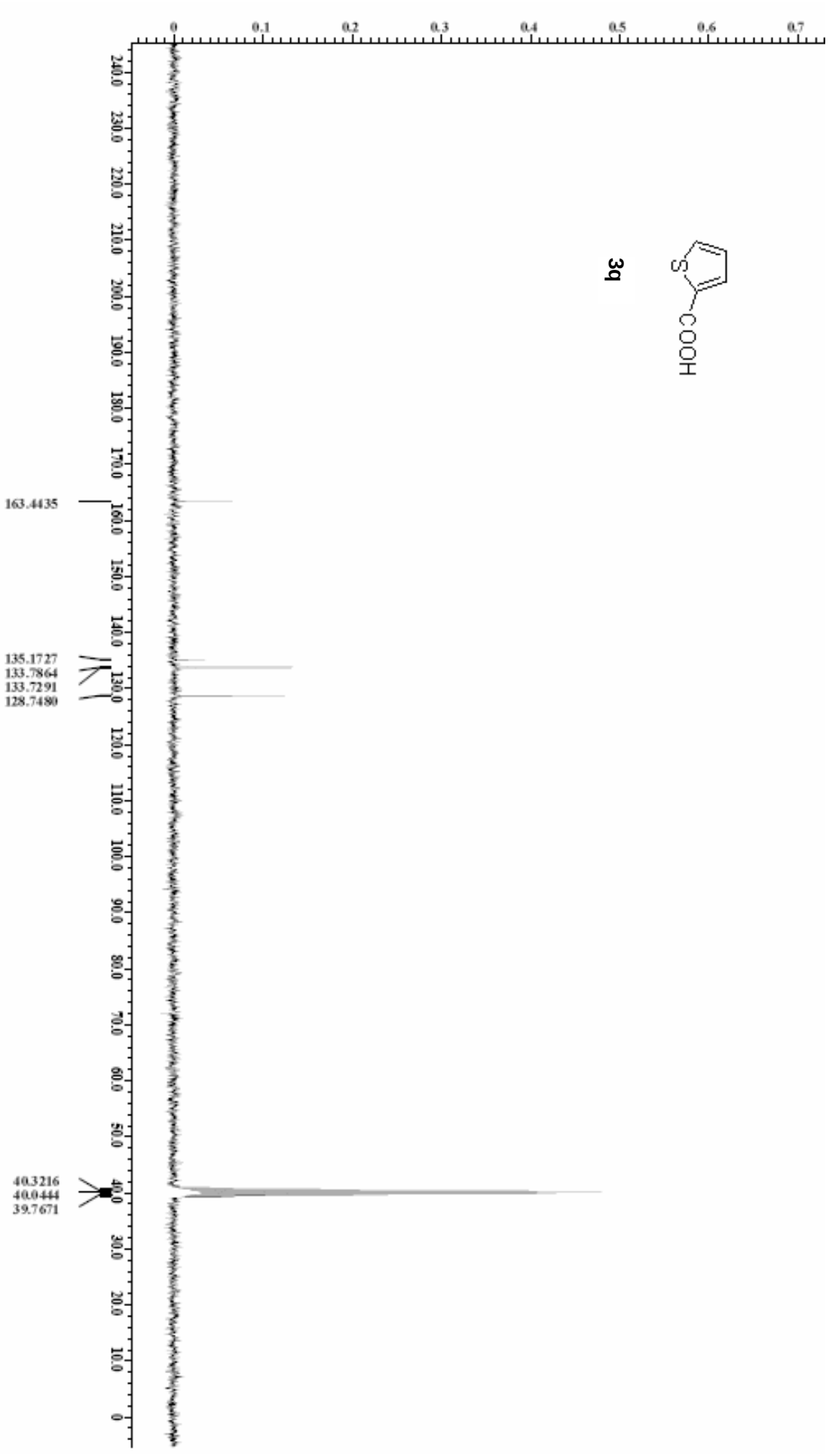
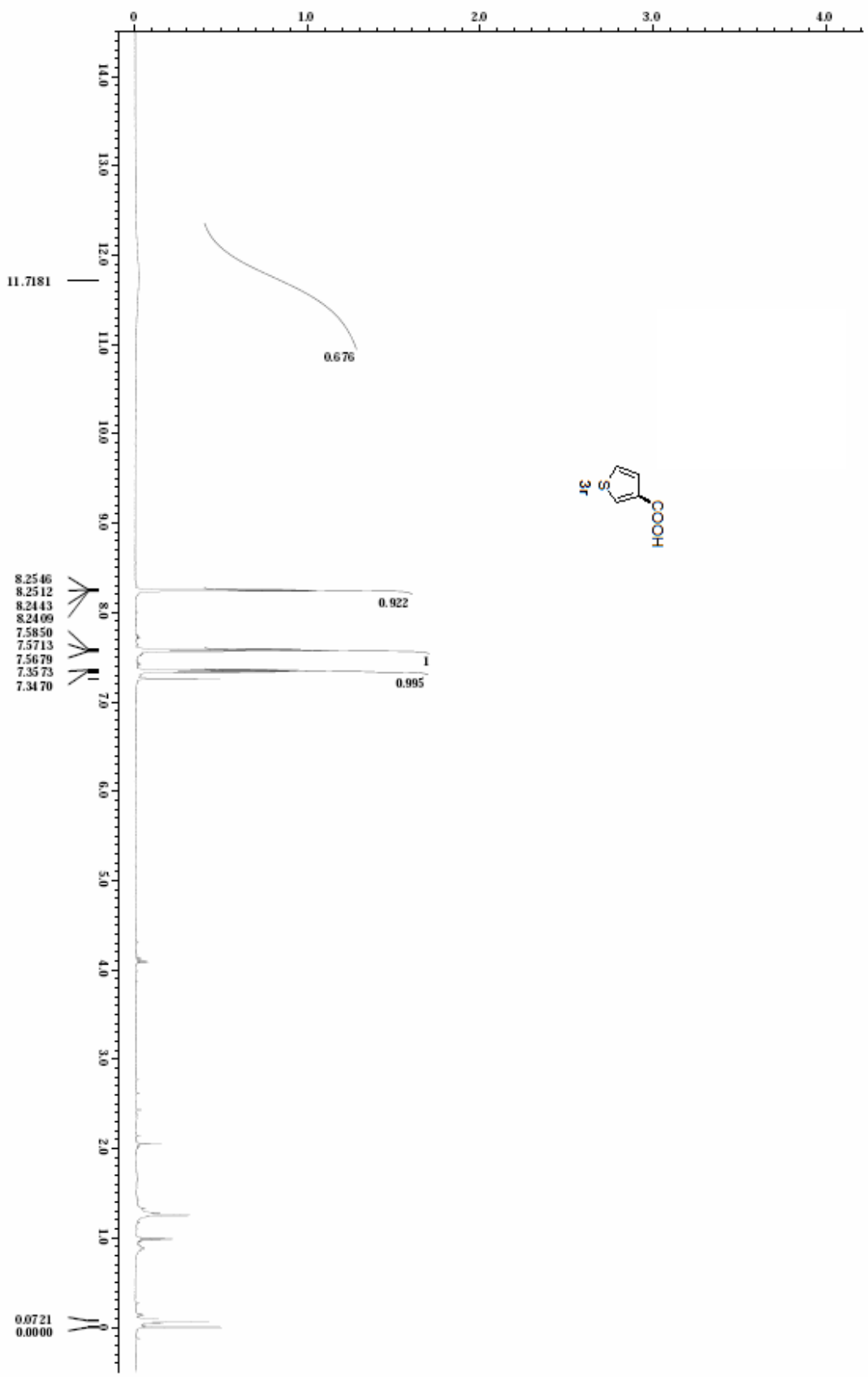
3.3799
2.5100
-0.0000
1.043
1.093
1.102
3g
S
COOH


3q
S
COOH
163.4435
135.1727
133.7864
133.7291
128.7480
40.3216
40.0444
39.7671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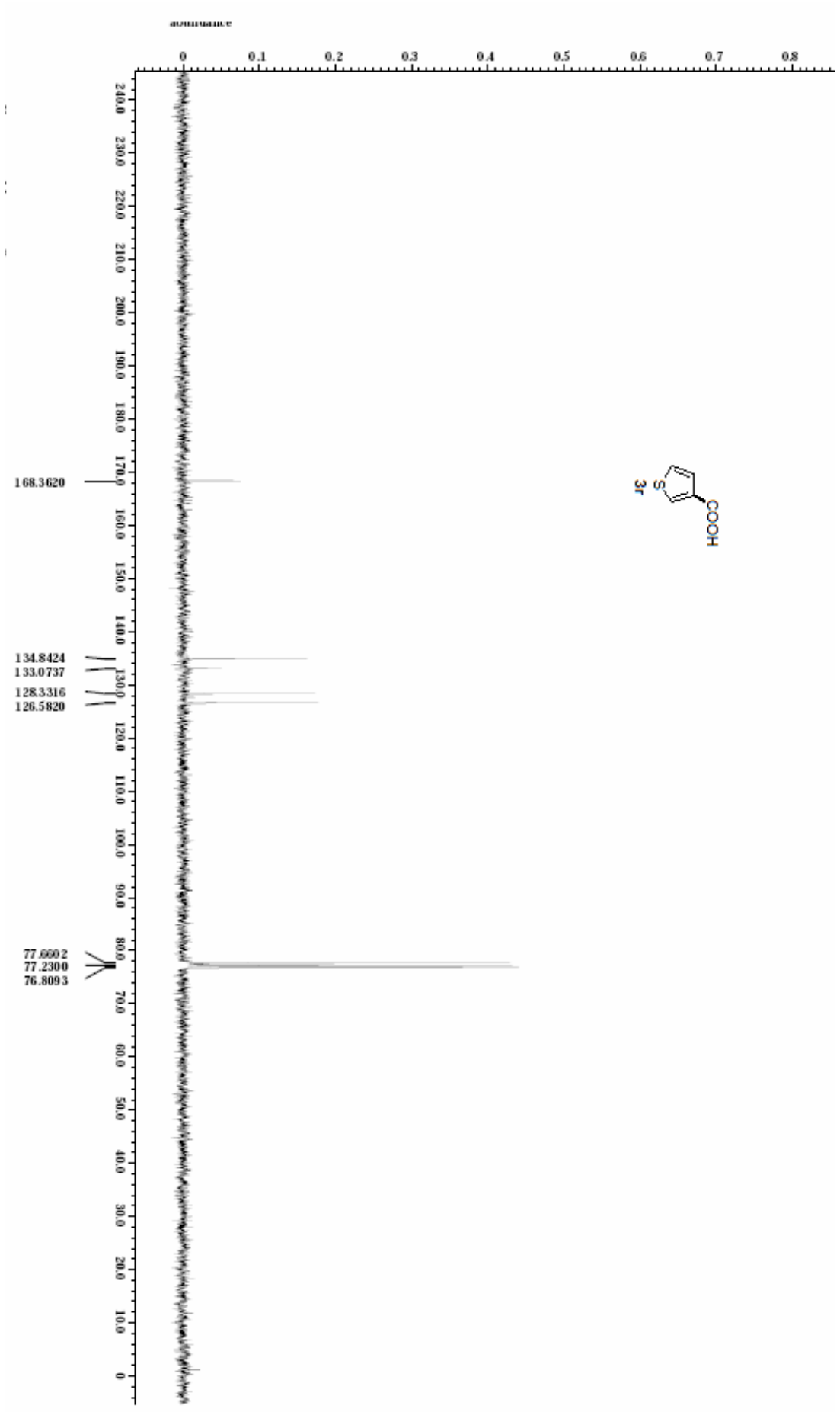
COOH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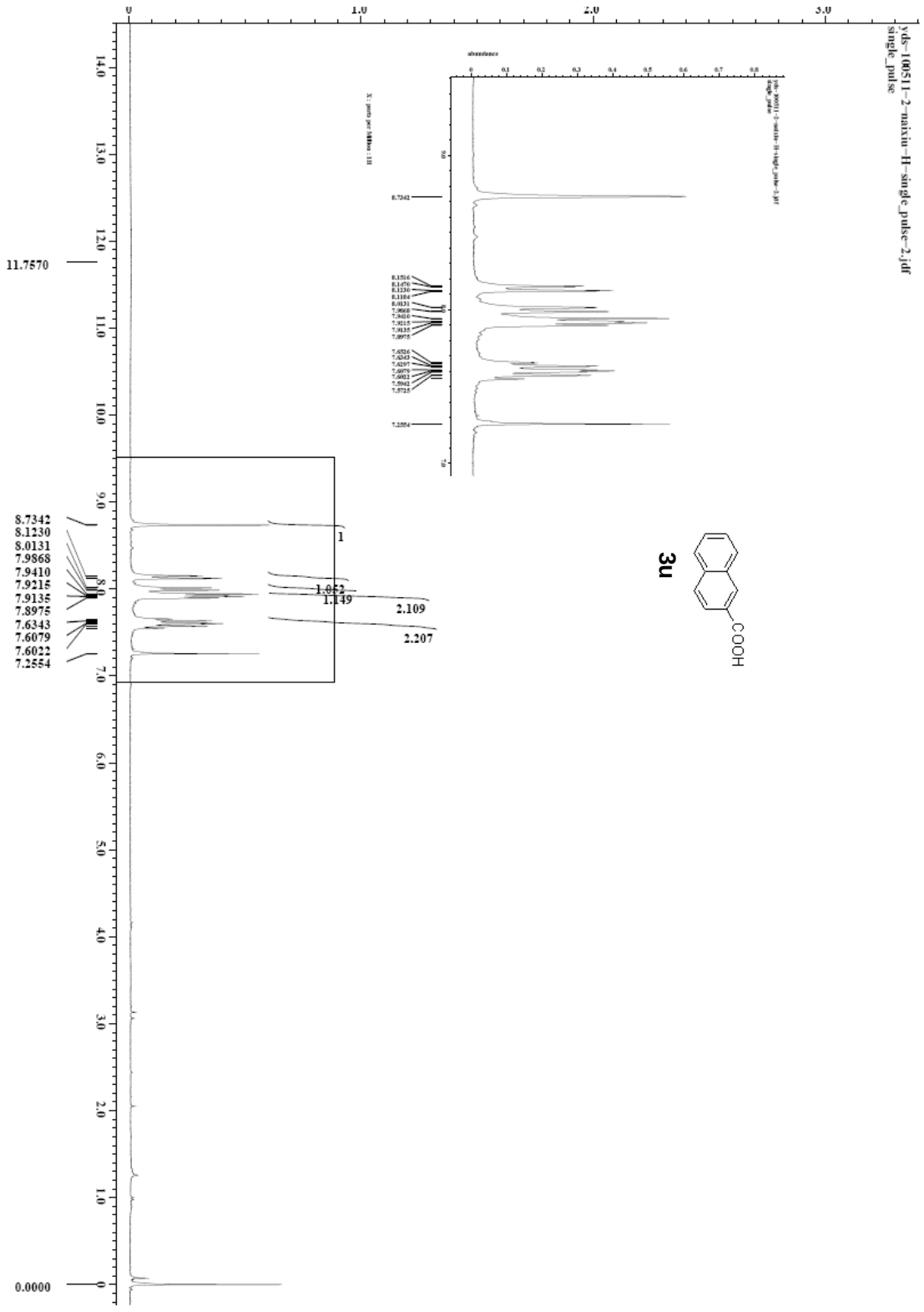
Br
S
HOOC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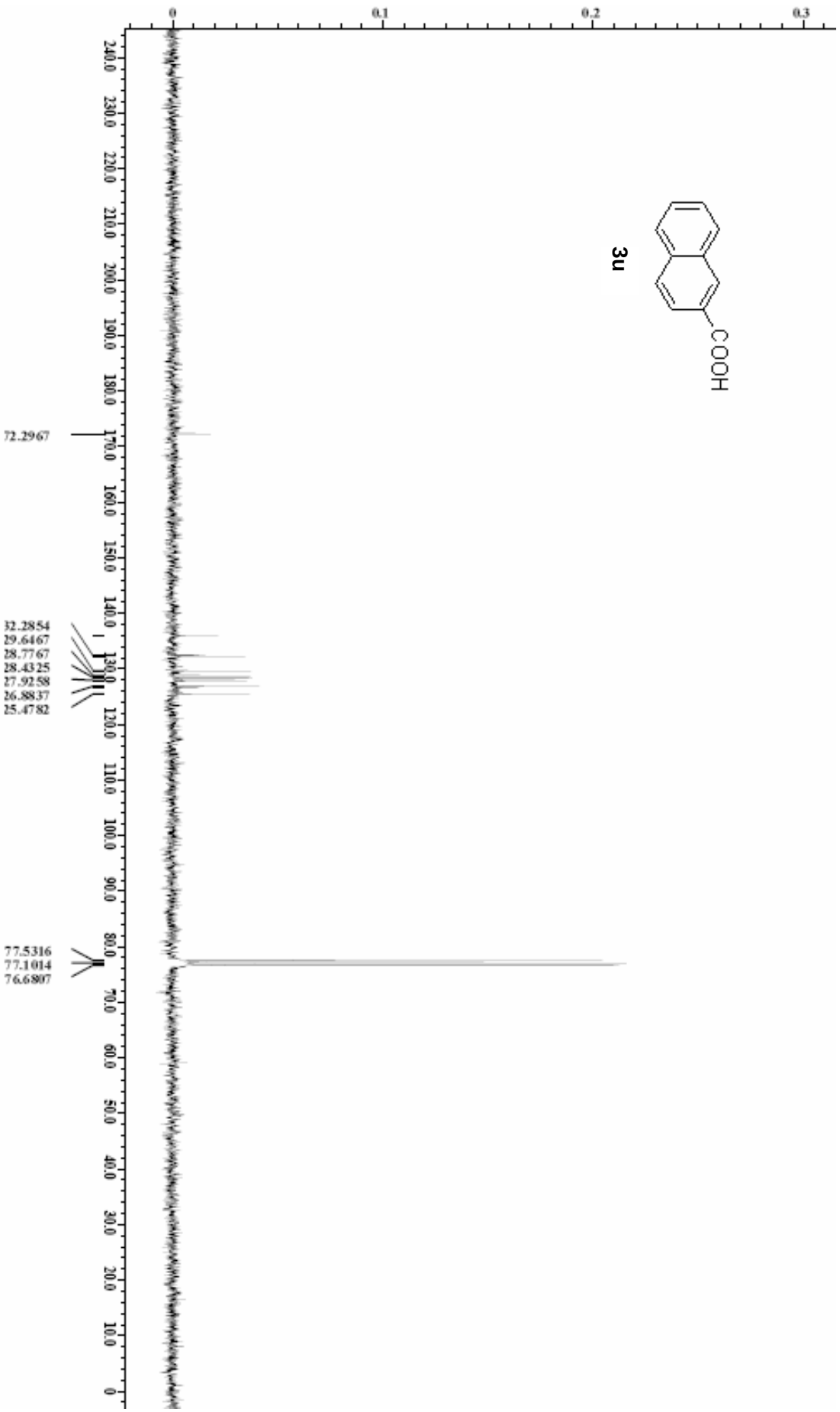
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